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* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS	1		Web Page URLs for STN Seminar Schedule - N. America
NEWS	2		"Ask CAS" for self-help around the clock
NEWS	3	SEP 09	CA/CAplus records now contain indexing from 1907 to the present
NEWS	4	Jul 15	Data from 1960-1976 added to RDISCLOSURE
NEWS	5	Jul 21	Identification of STN records implemented
NEWS	6	Jul 21	Polymer class term count added to REGISTRY
NEWS	7	Jul 22	INPADOC: Basic index (/BI) enhanced; Simultaneous Left and Right Truncation available
NEWS	8	AUG 05	New pricing for EUROPATFULL and PCTFULL effective August 1, 2003
NEWS	9	AUG 13	Field Availability (/FA) field enhanced in BEILSTEIN
NEWS	10	AUG 15	PATDPAFULL: one FREE connect hour, per account, in September 2003
NEWS	11	AUG 15	PCTGEN: one FREE connect hour, per account, in September 2003
NEWS	12	AUG 15	RDISCLOSURE: one FREE connect hour, per account, in September 2003
NEWS	13	AUG 15	TEMA: one FREE connect hour, per account, in September 2003
NEWS	14	AUG 18	Data available for download as a PDF in RDISCLOSURE
NEWS	15	AUG 18	Simultaneous left and right truncation added to PASCAL
NEWS	16	AUG 18	FROSTI and KOSMET enhanced with Simultaneous Left and Righ Truncation
NEWS	17	AUG 18	Simultaneous left and right truncation added to ANABSTR
NEWS	18	SEP 22	DIPPR file reloaded
NEWS	19	SEP 25	INPADOC: Legal Status data to be reloaded
NEWS	20	SEP 29	DISSABS now available on STN

NEWS EXPRESS	April 4 CURRENT WINDOWS VERSION IS V6.01a, CURRENT MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP), AND CURRENT DISCOVER FILE IS DATED 01 APRIL 2003
NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS INTER	General Internet Information
NEWS LOGIN	Welcome Banner and News Items
NEWS PHONE	Direct Dial and Telecommunication Network Access to STN
NEWS WWW	CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

* * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

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FILE 'HOME' ENTERED AT 16:27:17 ON 29 SEP 2003

=> file .biotech
COST IN U.S. DOLLARS                                    SINCE FILE      TOTAL
                                                           ENTRY    SESSION
FULL ESTIMATED COST                                         0.21       0.21

FILE 'MEDLINE' ENTERED AT 16:27:32 ON 29 SEP 2003

FILE 'BIOSIS' ENTERED AT 16:27:32 ON 29 SEP 2003
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FILE 'BIOTECHDS' ENTERED AT 16:27:32 ON 29 SEP 2003
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FILE 'CAPLUS' ENTERED AT 16:27:32 ON 29 SEP 2003
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=> s QSPR
L1         1391 QSPR

=> s 2d fingerprint
L2           14 2D FINGERPRINT

=> s l1 and l2
L3            2 L1 AND L2

=> d ti l2

L2   ANSWER 1 OF 14      MEDLINE on STN
TI   Measuring molecular similarity and diversity: total pharmacophore
     diversity.


=> d ti l2 1-14

L2   ANSWER 1 OF 14      MEDLINE on STN
TI   Measuring molecular similarity and diversity: total pharmacophore
     diversity.

L2   ANSWER 2 OF 14      MEDLINE on STN
TI   Database searching for compounds with similar biological activity using
     short binary bit string representations of molecules.

L2   ANSWER 3 OF 14      MEDLINE on STN
TI   FLEXS: a method for fast flexible ligand superposition.

L2   ANSWER 4 OF 14  BIOSIS  COPYRIGHT 2003 BIOLOGICAL ABSTRACTS INC. on STN
TI   Measuring molecular similarity and diversity: Total pharmacophore
     diversity.

L2   ANSWER 5 OF 14  BIOSIS  COPYRIGHT 2003 BIOLOGICAL ABSTRACTS INC. on STN
TI   FlexS: A method for fast flexible ligand superposition.

L2   ANSWER 6 OF 14  CAPLUS  COPYRIGHT 2003 ACS on STN
TI   Method and system for predicting pharmacokinetic properties

L2   ANSWER 7 OF 14  CAPLUS  COPYRIGHT 2003 ACS on STN
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TI Measuring molecular similarity and diversity: total pharmacophore diversity

L2 ANSWER 8 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN
TI Comparison of **2D fingerprint** types and hierarchy level selection methods for structural grouping using Ward's clustering

L2 ANSWER 9 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN
TI Comparing 3D Pharmacophore Triplets and 2D Fingerprints for Selecting Diverse Compound Subsets

L2 ANSWER 10 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN
TI Database searching for compounds with similar biological activity using short binary bit string representations of molecules

L2 ANSWER 11 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN
TI Accurate prediction of solvation free energy and lipophilicity of organic molecules using atomic constants and fingerprints

L2 ANSWER 12 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN
TI FLEXS: A Method for Fast Flexible Ligand Superposition

L2 ANSWER 13 OF 14 EMBASE COPYRIGHT 2003 ELSEVIER INC. ALL RIGHTS RESERVED. on STN
TI Measuring molecular similarity and diversity: Total pharmacophore diversity.

L2 ANSWER 14 OF 14 EMBASE COPYRIGHT 2003 ELSEVIER INC. ALL RIGHTS RESERVED. on STN
TI FLEXS: A method for fast flexible ligand superposition.

=> d ibib abs l2 11

L2 ANSWER 11 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1999:146813 CAPLUS
TITLE: Accurate prediction of solvation free energy and lipophilicity of organic molecules using atomic constants and fingerprints
AUTHOR(S): Viswanadhan, Vellarkad N.; Ghose, Arup K.; Singh, U. C.; Wendoloski, John J.
CORPORATE SOURCE: Amgen Inc., Thousand Oaks, CA, 91320, USA
SOURCE: Book of Abstracts, 217th ACS National Meeting, Anaheim, Calif., March 21-25 (1999), COMP-222. American Chemical Society: Washington, D. C. CODEN: 67GHA6
DOCUMENT TYPE: Conference; Meeting Abstract
LANGUAGE: English
AB Two additive-constitutive QSPR models are developed for the computation of solvation free energies and lipophilicity (Log P) of org. mols. using the ALOGP atom type definitions and mol. holograms based on 2D-fingerprints of compds. Mol. holograms - a special form of 2D fingerprints - encode more information than a traditional **2D fingerprint**, by retaining counts of unique fragments. The QSPR models for the solvation free energy are developed from a database of 265 org. mols. The Log P models were developed on a database of about 9000 compds. For the test sets, both models are shown to be highly predictive. The hologram approach is shown to be effective for the prediction of Log P, though the at. const. method (using the ALOGP atom types) gives better results.

=> d ibib abs l3 1-2

L3 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2002:10123 CAPLUS
DOCUMENT NUMBER: 136:64091
TITLE: Method and system for predicting pharmacokinetic properties
INVENTOR(S): Hattori, Kazunari; Shimada, Kaore; Uchiyama, Mamoru
PATENT ASSIGNEE(S): Pfizer Inc., USA
SOURCE: Eur. Pat. Appl., 27 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1167969	A2	20020102	EP 2001-304648	20010525
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
US 2003069698	A1	20030410	US 2001-876767	20010607
JP 2003014728	A2	20030115	JP 2001-179774	20010614

PRIORITY APPLN. INFO.: US 2000-211864P P 20000614

AB This invention provides a method for predicting pharmacokinetic properties of mols. comprising the steps of: (a) prepg. 2D-structures of mols. used as a training set; (b) constructing a **2D-fingerprint** by counting the no. of structural descriptors that potentially relate to a pharmacokinetic property, either manually or automatically using internally developed macro; wherein said structural descriptors consist of predefined 20 to 80 atoms/fragments or substructures; (c) analyzing the obtained **2D-fingerprint** by a statistical anal. method to correlate with the pharmacokinetic property of the mol. to yield a quant. structure-property relation (**QSPR**) model; and (d) calcg. the pharmacokinetic property of a trial mol. using the above obtained **QSPR** model. A system for this invention is also provided. According to this method and system, it is possible to predict pharmacokinetic properties of mols. prior to synthesis, without labor-intensive and time-consuming experimentation.

L3 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1999:146813 CAPLUS
TITLE: Accurate prediction of solvation free energy and lipophilicity of organic molecules using atomic constants and fingerprints
AUTHOR(S): Viswanadhan, Vellarkad N.; Ghose, Arup K.; Singh, U. C.; Wendoloski, John J.
CORPORATE SOURCE: Amgen Inc., Thousand Oaks, CA, 91320, USA
SOURCE: Book of Abstracts, 217th ACS National Meeting, Anaheim, Calif., March 21-25 (1999), COMP-222. American Chemical Society: Washington, D. C.
CODEN: 67GHA6
DOCUMENT TYPE: Conference; Meeting Abstract
LANGUAGE: English

AB Two additive-constitutive **QSPR** models are developed for the computation of solvation free energies and lipophilicity (Log P) of org. mols. using the ALOGP atom type definitions and mol. holograms based on 2D-fingerprints of compds. Mol. holograms - a special form of 2D fingerprints - encode more information than a traditional **2D fingerprint**, by retaining counts of unique fragments. The **QSPR** models for the solvation free energy are developed from a database of 265 org. mols. The Log P models were developed on a database of about 9000 compds. For the test sets, both models are shown to be highly predictive. The hologram approach is shown to be effective for the prediction of Log P, though the at. const. method (using the ALOGP atom types) gives better results.

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=> d his

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     FILE 'MEDLINE, BIOSIS, BIOTECHDS, CAPLUS, EMBASE' ENTERED AT 16:27:32 ON
     29 SEP 2003
L1          1391 S QSPR
L2            14 S 2D FINGERPRINT
L3             2 S L1 AND L2

=> s 2d structure
L4          189 2D STRUCTURE

=> s l1 and l4
L5            0 L1 AND L4

=> s pharmacokinetic
L6       142325 PHARMACOKINETIC

=> s l4 and l6
L7            0 L4 AND L6

=> s adme
L8          649 ADME

=> s l4 and l8
L9            1 L4 AND L8

=> d ti l9

L9   ANSWER 1 OF 1  CAPLUS  COPYRIGHT 2003 ACS on STN
TI   High-throughput prediction of passive ADME properties from
     fragments


=> d ibib abs l9

L9   ANSWER 1 OF 1  CAPLUS  COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER:         2002:615971  CAPLUS
TITLE:                    High-throughput prediction of passive ADME
                          properties from fragments
AUTHOR(S):                Oprea, Tudor I.; Baroni, Massimo; Zamora, Ismael;
                          Cruciani, Gabriele
CORPORATE SOURCE:         EST Chemical Computing, AstraZeneca, Moelndal,
                          S-43183, Swed.
SOURCE:                   Abstracts of Papers, 224th ACS National Meeting,
                          Boston, MA, United States, August 18-22, 2002 (2002),
                          COMP-109.  American Chemical Society: Washington, D.
                          C.
                          CODEN: 69CZPZ
DOCUMENT TYPE:            Conference; Meeting Abstract
LANGUAGE:                 English
AB   Based on the GRID [1], VolSurf [2], ChemGPS [3] and GPSVS [4]
     technologies, PENGUINS (Pharmacokinetics Evaluation aNd GRID Utilization
     IN Silico) is designed to manipulate large nos. of compds. starting from
     2D structure.  In PENGUINS, one can use SMILES or SDF
     files, in the absence of 3D structures, to predict VolSurf parameters for
     the water and DRY probes, as well as GPSVS scores.  A precomputed database
     of fragments can be used to recognize input mols.  PENGUINS has the
     ability to provide fast and accurate predictions for virtual and/or
     existing chem. libraries, with respect to passive ADME
     properties such as oral (intestinal) drug absorption and blood-brain
     barrier drug permeation, as well as water soly. for more than one million
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compds. per CPU/day.

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=> s adsorption or distribution or metabolism or exretion
L10    6895655 ADSORPTION OR DISTRIBUTION OR METABOLISM OR EXRETION

=> s l1 and l10
L11         119 L1 AND L10

=> s l4 and l10
L12          28 L4 AND L10

=> d ti l12 1-28

L12  ANSWER 1 OF 28      MEDLINE on STN
TI   A Janus splicing regulatory element modulates HIV-1 tat and rev mRNA
     production by coordination of hnRNP A1 cooperative binding.

L12  ANSWER 2 OF 28      MEDLINE on STN
TI   CoMFA-based prediction of agonist affinities at recombinant wild type
     versus serine to alanine point mutated D2 dopamine receptors.

L12  ANSWER 3 OF 28      MEDLINE on STN
TI   An essential non-Watson-Crick base pair motif in 3'UTR to mediate
     selenoprotein translation.

L12  ANSWER 4 OF 28      MEDLINE on STN
TI   RNAs mediating cotranslational insertion of selenocysteine in eukaryotic
     selenoproteins.

L12  ANSWER 5 OF 28  BIOSIS  COPYRIGHT 2003 BIOLOGICAL ABSTRACTS INC. on STN
TI   Simulation of the 3D morphology of motoneuron dendrites.

L12  ANSWER 6 OF 28  CAPLUS  COPYRIGHT 2003 ACS on STN
TI   Novel nanosheet crystallites and their layer-by-layer assembly

L12  ANSWER 7 OF 28  CAPLUS  COPYRIGHT 2003 ACS on STN
TI   Analytical modelling of steady-state temperature distribution in
     thermal microsensors using Fourier method. Part 2. Practical application

L12  ANSWER 8 OF 28  CAPLUS  COPYRIGHT 2003 ACS on STN
TI   Analytical modelling of steady-state temperature distribution in
     thermal microsensors using Fourier method. Part 1. Theory

L12  ANSWER 9 OF 28  CAPLUS  COPYRIGHT 2003 ACS on STN
TI   STM observations of 2D Kr and Xe adsorbed on graphite

L12  ANSWER 10 OF 28  CAPLUS  COPYRIGHT 2003 ACS on STN
TI   New method for simulating charging effects on specimens in electron beam
     testing

L12  ANSWER 11 OF 28  CAPLUS  COPYRIGHT 2003 ACS on STN
TI   Two-Dimensional Structure of Self-Assembled Alkyl-Substituted
     Polyphenylene Dendrimers on Graphite

L12  ANSWER 12 OF 28  CAPLUS  COPYRIGHT 2003 ACS on STN
TI   Activation of Mg-based hydrogen storage materials modified by graphite and
     other carbonaceous compounds

L12  ANSWER 13 OF 28  CAPLUS  COPYRIGHT 2003 ACS on STN
TI   Scanning tunneling microscopy investigation of the ordered structures of
     dialkylamino hydroxylated squaraines adsorbed on highly oriented pyrolytic
     graphite. [Erratum to document cited in CA132:227939]
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L12 ANSWER 14 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN
TI Surface morphology development during ion sputtering. A IIIBV case

L12 ANSWER 15 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN
TI Analysis of the local conformation of proteins with two-dimensional fluorescence techniques

L12 ANSWER 16 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN
TI Scanning Tunneling Microscopy Investigation of the Ordered Structures of Dialkylamino Hydroxylated Squaraines Adsorbed on Highly Oriented Pyrolytic Graphite

L12 ANSWER 17 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN
TI A two-dimensional structure factor calculation for the Cu-1 plane in YBa2Cu3O6

L12 ANSWER 18 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN
TI Electrochemical construction of ultrathin film composed of quasi two-dimensional porphyrin polymers

L12 ANSWER 19 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN
TI The second half of the genetic code

L12 ANSWER 20 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN
TI Modeling of Ir adatoms on Ir surfaces

L12 ANSWER 21 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN
TI Effect of cobalt substitution on cationic **distribution** in LiNi1-yCoyO2 electrode materials

L12 ANSWER 22 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN
TI Orientation of grains boundaries in one- and two-dimensional polycrystals of aluminum.

L12 ANSWER 23 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN
TI Rapid control of the iron-garnet epitaxial films

L12 ANSWER 24 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN
TI Revisiting the iterative procedure for atomic beam diffraction analyses: improvements, caveats and first application to a 2D **adsorption** structure

L12 ANSWER 25 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN
TI Structural anomaly of liquid tin layers adsorbed on germanium(1 1 1) surfaces

L12 ANSWER 26 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN
TI Statistics of ion **distribution** in 1D and 2D mixed crystals

L12 ANSWER 27 OF 28 EMBASE COPYRIGHT 2003 ELSEVIER INC. ALL RIGHTS RESERVED. on STN
TI H-bridged structures for tetrahedranes A4H4 (A = C, Si, Ge, Sn, and Pb).

L12 ANSWER 28 OF 28 EMBASE COPYRIGHT 2003 ELSEVIER INC. ALL RIGHTS RESERVED. on STN
TI RNAs mediating cotranslational insertion of selenocysteine in eukaryotic selenoproteins.

=> d ti l11 1-20

L11 ANSWER 1 OF 119 MEDLINE on STN
TI Predicting drug pharmacokinetic properties using molecular interaction fields and SIMCA.

L11 ANSWER 2 OF 119 MEDLINE on STN
TI **QSPR**-based prediction of **adsorption** of halogenated aromatics on yellow-brown soil.

L11 ANSWER 3 OF 119 MEDLINE on STN
TI Development and validation of k-nearest-neighbor **QSPR** models of metabolic stability of drug candidates.

L11 ANSWER 4 OF 119 MEDLINE on STN
TI Quantum-mechanical QSAR/**QSPR** descriptors from momentum-space wave functions.

L11 ANSWER 5 OF 119 MEDLINE on STN
TI Prediction of vapour pressures for halogenated diphenyl ether congeners from molecular descriptors.

L11 ANSWER 6 OF 119 MEDLINE on STN
TI An approach to the interpretation of backpropagation neural network models in QSAR studies.

L11 ANSWER 7 OF 119 MEDLINE on STN
TI Molecular descriptors that influence the amount of drugs transfer into human breast milk.

L11 ANSWER 8 OF 119 MEDLINE on STN
TI Quantitative structure-permeability relationships (QSPRs) for percutaneous absorption.

L11 ANSWER 9 OF 119 MEDLINE on STN
TI An alignment-independent versatile structure descriptor for QSAR and **QSPR** based on the **distribution** of molecular features.

L11 ANSWER 10 OF 119 MEDLINE on STN
TI Prediction of Henry's law constants by a quantitative structure property relationship and neural networks.

L11 ANSWER 11 OF 119 MEDLINE on STN
TI Quantitative structure-pharmacokinetic relationship modelling.

L11 ANSWER 12 OF 119 MEDLINE on STN
TI Control of metalloprotein reduction potential: the role of electrostatic and solvation effects probed on plastocyanin mutants.

L11 ANSWER 13 OF 119 MEDLINE on STN
TI Structure-property relationships on histamine H3-antagonists: binding of phenyl-substituted alkylthioimidazole derivatives to rat plasma proteins.

L11 ANSWER 14 OF 119 MEDLINE on STN
TI Electronic eigenvalue (EEVA): a new QSAR/**QSPR** descriptor for electronic substituent effects based on molecular orbital energies. A QSAR approach to the Ah receptor binding affinity of polychlorinated biphenyls (PCBs), dibenzo-p-dioxins (PCDDs) and dibenzofurans (PCDFs).

L11 ANSWER 15 OF 119 MEDLINE on STN
TI Caco-2 cell permeability vs human gastrointestinal absorption: **QSPR** analysis.

L11 ANSWER 16 OF 119 MEDLINE on STN
TI **QSPR** correlation and predictions of GC retention indexes for methyl-branched hydrocarbons produced by insects.

L11 ANSWER 17 OF 119 MEDLINE on STN
TI Investigation of the mechanism of flux across human skin in vitro by

quantitative structure-permeability relationships.

L11 ANSWER 18 OF 119 MEDLINE on STN
TI Development of quantitative structure-pharmacokinetic relationships.

L11 ANSWER 19 OF 119 BIOSIS COPYRIGHT 2003 BIOLOGICAL ABSTRACTS INC. on STN
TI Development and validation of k-nearest-neighbor **QSPR** models of metabolic stability of drug candidates.

L11 ANSWER 20 OF 119 BIOSIS COPYRIGHT 2003 BIOLOGICAL ABSTRACTS INC. on STN
TI **QSPR**-based prediction of **adsorption** of halogenated aromatics on yellow-brown soil.

=> s l11 not py>2000
L13 46 L11 NOT PY>2000

=> dup rem l13
PROCESSING COMPLETED FOR L13
L14 37 DUP REM L13 (9 DUPLICATES REMOVED)

=> d ti l14 1-37

L14 ANSWER 1 OF 37 CAPLUS COPYRIGHT 2003 ACS on STN
TI Stability of Complexes of Aromatic Amides with Bromide Anion: Quantitative Structure-Property Relationships

L14 ANSWER 2 OF 37 MEDLINE on STN
TI Electronic eigenvalue (EEVA): a new QSAR/**QSPR** descriptor for electronic substituent effects based on molecular orbital energies. A QSAR approach to the Ah receptor binding affinity of polychlorinated biphenyls (PCBs), dibenzo-p-dioxins (PCDDs) and dibenzofurans (PCDFs).

L14 ANSWER 3 OF 37 CAPLUS COPYRIGHT 2003 ACS on STN
TI Estimation of hydrophobicity using quasi-molecular volume of quarternary ammonium ions

L14 ANSWER 4 OF 37 CAPLUS COPYRIGHT 2003 ACS on STN
TI Sorption study of substituted aromatic ketone in soil by batch equilibrium method

L14 ANSWER 5 OF 37 CAPLUS COPYRIGHT 2003 ACS on STN
TI **QSPR** of interfacial phenomena of 8-sulfonamidoquinolines

L14 ANSWER 6 OF 37 CAPLUS COPYRIGHT 2003 ACS on STN
TI Prediction of partition properties of substituted benzaldehydes using different structural parameters

L14 ANSWER 7 OF 37 CAPLUS COPYRIGHT 2003 ACS on STN
TI **QSPR** prediction of Henry's law constant: improved correlation with new parameters

L14 ANSWER 8 OF 37 MEDLINE on STN
TI Structure-property relationships on histamine H3-antagonists: binding of phenyl-substituted alkylthioimidazole derivatives to rat plasma proteins.

L14 ANSWER 9 OF 37 CAPLUS COPYRIGHT 2003 ACS on STN
TI Numerical drug-fitness index.

L14 ANSWER 10 OF 37 MEDLINE on STN
TI **QSPR** correlation and predictions of GC retention indexes for methyl-branched hydrocarbons produced by insects.

L14 ANSWER 11 OF 37 CAPLUS COPYRIGHT 2003 ACS on STN DUPLICATE 1

TI A new 3D molecular structure representation using quantum topology with application to structure-property relationships

L14 ANSWER 12 OF 37 CAPLUS COPYRIGHT 2003 ACS on STN
TI A review of QSAR for dye affinity for cellulose fibres

L14 ANSWER 13 OF 37 MEDLINE on STN DUPLICATE 2
TI Caco-2 cell permeability vs human gastrointestinal absorption: **QSPR** analysis.

L14 ANSWER 14 OF 37 BIOSIS COPYRIGHT 2003 BIOLOGICAL ABSTRACTS INC. on STN DUPLICATE 3
TI Quantitative structure-property relationship (**QSPR**) for the **adsorption** of organic compounds onto activated carbon cloth: Comparison between multiple linear regression and neural network.

L14 ANSWER 15 OF 37 CAPLUS COPYRIGHT 2003 ACS on STN
TI Determination and **QSPR** analysis of log Kow and log Koc for fluorine containing benzene derivatives

L14 ANSWER 16 OF 37 MEDLINE on STN
TI Investigation of the mechanism of flux across human skin in vitro by quantitative structure-permeability relationships.

L14 ANSWER 17 OF 37 CAPLUS COPYRIGHT 2003 ACS on STN
TI Solvent extraction and **QSPR** of catecholamines with a bis(2-ethylhexyl) hydrogen phosphate

L14 ANSWER 18 OF 37 CAPLUS COPYRIGHT 2003 ACS on STN
TI Using AM1 hamiltonian in prediction of benzaldehydes sorption on soil

L14 ANSWER 19 OF 37 CAPLUS COPYRIGHT 2003 ACS on STN
TI Improved valence connectivity topological index and its application - .delta.i- comparison with .delta.v in QSAR/**QSPR** of three systems

L14 ANSWER 20 OF 37 CAPLUS COPYRIGHT 2003 ACS on STN
TI Evaluation and use of BCUT descriptors in QSAR and **QSPR** studies.

L14 ANSWER 21 OF 37 CAPLUS COPYRIGHT 2003 ACS on STN
TI Quantitative structure-retention relationship study of tetrazolium salts on alumina support

L14 ANSWER 22 OF 37 CAPLUS COPYRIGHT 2003 ACS on STN DUPLICATE 4
TI 3D-modeling and prediction by WHIM descriptors. Part 9. Chromatographic relative retention time and physico-chemical properties of polychlorinated biphenyls (PCBs)

L14 ANSWER 23 OF 37 BIOSIS COPYRIGHT 2003 BIOLOGICAL ABSTRACTS INC. on STN
TI Quantitative structure property relationships (**QSPR**) for prediction of solution **adsorption** process parameters using fumed silica.

L14 ANSWER 24 OF 37 EMBASE COPYRIGHT 2003 ELSEVIER INC. ALL RIGHTS RESERVED. on STN
TI Prediction of the soil sorption coefficient of organic pollutants by the characteristic root index model.

L14 ANSWER 25 OF 37 BIOSIS COPYRIGHT 2003 BIOLOGICAL ABSTRACTS INC. on STN DUPLICATE 5
TI **Adsorption** behaviour and **QSPR** studies of organotin compounds on estuarine sediment.

L14 ANSWER 26 OF 37 CAPLUS COPYRIGHT 2003 ACS on STN
TI Use of semiempirical quantum-chemical molecular descriptors in QSAR

QSPR.

L14 ANSWER 27 OF 37 CAPLUS COPYRIGHT 2003 ACS on STN
TI Rotational barrier of the polychlorinated biphenyls as a physicochemical parameter for use in modeling of QSARs and QSPRs

L14 ANSWER 28 OF 37 CAPLUS COPYRIGHT 2003 ACS on STN
TI **QSPR** and GCA Models for Predicting the Normal Boiling Points of Fluorocarbons

L14 ANSWER 29 OF 37 BIOSIS COPYRIGHT 2003 BIOLOGICAL ABSTRACTS INC. on STN DUPLICATE 6
TI Quantitative structure-pharmacokinetics relationships (**QSPR**) of beta blockers derived using neural networks.

L14 ANSWER 30 OF 37 CAPLUS COPYRIGHT 2003 ACS on STN
TI Prediction of surface tension of organic liquids

L14 ANSWER 31 OF 37 BIOSIS COPYRIGHT 2003 BIOLOGICAL ABSTRACTS INC. on STN
TI **QSPR** and QSAR study of phthalimidohydroxamic acids.

L14 ANSWER 32 OF 37 CAPLUS COPYRIGHT 2003 ACS on STN
TI Theory and software for a general model of solute-solvent interactions.

L14 ANSWER 33 OF 37 BIOSIS COPYRIGHT 2003 BIOLOGICAL ABSTRACTS INC. on STN
TI A comparative study of some topological indices and log P in structure-property-activity analysis of phenylalkylamines.

L14 ANSWER 34 OF 37 CAPLUS COPYRIGHT 2003 ACS on STN DUPLICATE 7
TI Predictive **QSPR** models for estimating soil sorption coefficients: potential and limitations based on dominating processes

L14 ANSWER 35 OF 37 CAPLUS COPYRIGHT 2003 ACS on STN
TI Quantitative structure - pharmacokinetic relationship (**QSPR**) analysis for arylalkanoic acid nonsteroidal anti-inflammatory drugs

L14 ANSWER 36 OF 37 CAPLUS COPYRIGHT 2003 ACS on STN
TI General methodology and computer program for the exhaustive restoring of chemical structures by molecular connectivity indexes. Solution of the inverse problem in QSAR/**QSPR**

L14 ANSWER 37 OF 37 MEDLINE on STN
TI Development of quantitative structure-pharmacokinetic relationships.

=> dup rem l11
PROCESSING COMPLETED FOR L11
L15 87 DUP REM L11 (32 DUPLICATES REMOVED)

=> d ibib abs l15 1-20

L15 ANSWER 1 OF 87 MEDLINE on STN DUPLICATE 1
ACCESSION NUMBER: 2003316291 MEDLINE
DOCUMENT NUMBER: 22710998 PubMed ID: 12825940
TITLE: Development and validation of k-nearest-neighbor **QSPR** models of metabolic stability of drug candidates.
AUTHOR: Shen Min; Xiao Yunde; Golbraikh Alexander; Gombar Vijay K; Tropsha Alexander
CORPORATE SOURCE: Division of Medicinal Chemistry and Natural Products, School of Pharmacy, CB# 7360, University of North Carolina, Chapel Hill, North Carolina 27599-7360, USA.
SOURCE: JOURNAL OF MEDICINAL CHEMISTRY, (2003 Jul 3) 46 (14) 3013-20.

Journal code: 9716531. ISSN: 0022-2623.
PUB. COUNTRY: United States
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE) (VALIDATION STUDIES)
LANGUAGE: English
FILE SEGMENT: Priority Journals
ENTRY MONTH: 200308
ENTRY DATE: Entered STN: 20030709
Last Updated on STN: 20030808
Entered Medline: 20030807

AB Computational ADME (absorption, **distribution**, **metabolism**, and excretion) models may be used early in the drug discovery process in order to flag drug candidates with potentially problematic ADME profiles. We report the development, validation, and application of quantitative structure-property relationship (**QSPR**) models of metabolic turnover rate for compounds in human S9 homogenate. Biological data were obtained from uniform bioassays of 631 diverse chemicals proprietary to GlaxoSmithKline (GSK). The models were built with topological molecular descriptors such as molecular connectivity indices or atom pairs using the k-nearest neighbor variable selection optimization method developed at the University of North Carolina (Zheng, W.; Tropsha, A. A novel variable selection QSAR approach based on the k-nearest neighbor principle. J. Chem. Inf. Comput. Sci., 2000, 40, 185-194.). For the purpose of validation, the whole data set was divided into training and test sets. The training set **QSPR** models were characterized by high internal accuracy with leave-one-out cross-validated R(2) (q(2)) values ranging between 0.5 and 0.6. The test set compounds were correctly classified as stable or unstable in S9 assay with an accuracy above 85%. These models were additionally validated by in silico metabolic stability screening of 107 new chemicals under development in several drug discovery programs at GSK. One representative model generated with MolConnZ descriptors predicted 40 compounds to be metabolically stable (turnover rate less than 25%), and 33 of them were indeed found to be stable experimentally. This success (83% concordance) in correctly picking chemicals that are metabolically stable in the human S9 homogenate spells a rapid, computational screen for generating components of the ADME profile in a drug discovery process.

L15 ANSWER 2 OF 87 BIOSIS COPYRIGHT 2003 BIOLOGICAL ABSTRACTS INC. on STN
ACCESSION NUMBER: 2003:242563 BIOSIS
DOCUMENT NUMBER: PREV200300242563
TITLE: Integrated **QSPR**: Pharmacodynamic model of genomic effects of several corticosteroids.
AUTHOR(S): Mager, Donald E.; Pyszczynski, Nancy A.; Jusko, William J. (1)
CORPORATE SOURCE: (1) Department of Pharmaceutical Sciences, School of Pharmacy and Pharmaceutical Sciences, University at Buffalo, State University of New York, Buffalo, NY, 14260, USA: wjjusko@buffalo.edu USA
SOURCE: Journal of Pharmaceutical Sciences, (April 2003, 2003) Vol. 92, No. 4, pp. 881-889. print.
ISSN: 0022-3549.
DOCUMENT TYPE: Article
LANGUAGE: English

AB The results from a quantitative structure-property relationship (**QSPR**) model was integrated into a fifth-generation pharmacokinetic/pharmacodynamic (PK/PD) model of corticosteroid receptor/gene-mediated effects. The proposed model was developed using previously reported tyrosine aminotransferase (TAT) activity data following a 50 mg/kg intravenous dose of methylprednisolone in male adrenalectomized (ADX) rats. Induced TAT activity is a classical measure of corticosteroid genomic effects and the typical time course shows an initial lag-time, a slow rise to peak response, and a gradual return toward baseline values. The TAT activity profiles were subsequently

predicted for two additional steroids (dexamethasone and hydrocortisone), which were confirmed experimentally. Two groups of male ADX Wistar rats (n = 18 each) were given either 0.1 mg/kg dexamethasone or 50 mg/kg hydrocortisone by penile vein injections. Plasma drug concentrations and liver TAT activity were measured at various time points. Baseline TAT activity was significantly lower in this study as compared to previous reports. Model simulations well captured the pharmacodynamic data once initial conditions were corrected for observed baseline values. Additional TAT profiles reported in the literature for prednisolone were also reasonably predicted using the final model. This study serves as a demonstration of how in vitro pharmacologic data and **QSPR** modeling results may be incorporated into existing mechanistic PK/PD models to anticipate the effects of other chemically related compounds.

L15 ANSWER 3 OF 87 MEDLINE on STN DUPLICATE 2
ACCESSION NUMBER: 2003139848 MEDLINE
DOCUMENT NUMBER: 22541701 PubMed ID: 12653520
TITLE: Quantum-mechanical QSAR/**QSPR** descriptors from momentum-space wave functions.
AUTHOR: McCoy Errol F; Sykes Matthew J
CORPORATE SOURCE: School of Chemistry, Physics and Earth Sciences, Flinders University, GPO Box 2100, Adelaide, SA, Australia 5001.
SOURCE: JOURNAL OF CHEMICAL INFORMATION AND COMPUTER SCIENCES, (2003 Mar-Apr) 43 (2) 545-53.
Journal code: 7505012. ISSN: 0095-2338.
PUB. COUNTRY: United States
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English
ENTRY MONTH: 200306
ENTRY DATE: Entered STN: 20030326
Last Updated on STN: 20030627
Entered Medline: 20030626

AB It is shown that quantum-mechanical descriptors obtained as parameters from the one-dimensional radial **distribution** function of electron momentum can be used to predict molecular activities or properties to a precision that compares favorably with the more traditional QSAR/**QSPR** methods. The **distribution** function is derived from momentum space ab initio wave functions. The predictive value of the descriptors is illustrated by their application to the estimation of McGowan's volume, gas-chromatographic retention time, gas-hexadecane partition coefficient, second hyperpolarizability, and tadpole narcotic activity.

L15 ANSWER 4 OF 87 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2003:481699 CAPLUS
DOCUMENT NUMBER: 139:164501
TITLE: Structural properties and photoreactivity relationships of substituted phenols in TiO2 suspensions
AUTHOR(S): Parra, S.; Olivero, J.; Pacheco, L.; Pulgarin, C.
CORPORATE SOURCE: ENAC, Laboratory of Environmental Biotechnology, Group of Coupled Chemical and Biological Processes, Swiss Federal Institute of Technology, EPFL, Lausanne, CH-1015, Switz.
SOURCE: Applied Catalysis, B: Environmental (2003), 43(3), 293-301
CODEN: ACBEE3; ISSN: 0926-3373
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The reactivity of phenolic compds. can be drastically affected by the electronic nature of substituents and by their positions in the arom. ring. In this work, structure effect on the photoreactivity via TiO2 catalysis is studied using several substituted phenols in order to cover a

wide variety of electronic effects, ranging from strong electron-donating (activating) to strong electron-withdrawing (deactivating) groups: -OH, -OCH3, -OCH2CH2CH3, -COOH, -COH, -COCH3, -NO2, -SO3H, -CN, -CF3, -F, -Cl, -Br, and -I.Results indicate that the fastest initial degrdn. rate for substituted phenols occurs for p-methoxyphenol and the slowest for the p-nitrophenol. Quantum chem. derived properties and exptl. data for each phenol deriv. were used to establish structure-photoreactivity relationships (SPR) for these compds. using regression techniques. According to the statistical calcns., the most crit. electronic properties responsible for the photoreactivity of p-substituted phenols were the zero-point energy, the total energy divided by the mol. wt., and the quadrupolar moment for the xy plane. These mol. descriptors encode information related to the mol. vibration frequencies, intra-mol. interactions, and total electron **distribution** around the mol., resp. This SPR approach offer a better explanation of the para-phenols photoreactivity properties than the use of Hammett const. because it considers properties derived from whole mols. whose atoms interact with the light based on the electron d. and electronic mol. shape.

REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 5 OF 87 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2003:664843 CAPLUS

DOCUMENT NUMBER: 139:169824

TITLE: Influence of VOCs molecular characteristics on exothermicity of **adsorption** onto activated carbon

AUTHOR(S): Pre, P.; Faur-Brasquet, C.; Le Cloirec, P.

CORPORATE SOURCE: Ecole des Mines de Nantes, GEPEA, UMR-CNRS 6144, Nantes, 44307, Fr.

SOURCE: Adsorption Science and Technology, Proceedings of the Pacific Basin Conference, 3rd, Kyongju, Republic of Korea, May 25-29, 2003 (2003), 264-269. Editor(s): Lee, Chang-Ha. World Scientific Publishing Co. Pte. Ltd.: Singapore, Singapore.
CODEN: 69EJHN; ISBN: 981-238-349-2

DOCUMENT TYPE: Conference

LANGUAGE: English

AB The objective of the study was to point out the influence of the mol. properties of volatile org. compds. (VOCs) on the intensity of the energetic interactions with activated C. The integral **adsorption** enthalpies of 44 org. species were first measured onto one type of granular activated C. Depending on the nature of the VOC, the **adsorption** enthalpy may vary from 40 to 80 kJ.mol-1. To account for the influence of the mol. properties on the variations obsd., quant. structure property relationships (QSPRs) were investigated. QSPRs were set up through different statistical approaches which enabled to discriminate the mol. characteristics which have a significant influence on the **adsorption** energy. Phys. data representative of both dimensional and electronic properties of the org. mols. were retained to form the input variable set. As a simplest tool, a multiple linear regression was first investigated. The best linear regression obtained involved 3 explicative variables: the ionization potential, the polarizability and the molar mass. The linear model permits to compute the **adsorption** energies by less than 15% in error. In a second approach, a non linear model was also attempted, using neural networks. According to the size of the exptl. database, the no. of neurons in the input layer was restricted to 3. The best neural network was selected after training was achieved with 56 input variable triplets. The same mol. properties previously involved in the linear regression, also merge in the best neural network. The predictive ability of the neural network is then proved to be comparable to that of the linear regression.

REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 6 OF 87 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2003:107629 CAPLUS
DOCUMENT NUMBER: 138:368358
TITLE: Theoretical calculation of isotope effects, kinetic energy release and effective temperatures for alkylamines
AUTHOR(S): Drahos, Laszlo; Sztaray, Judit; Vekey, Karoly
CORPORATE SOURCE: Chemical Research Center, Hungarian Academy of Sciences, Budapest, H-1025, Hung.
SOURCE: International Journal of Mass Spectrometry (2003), 225(3), 233-248
CODEN: IMSPF8; ISSN: 1387-3806
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The kinetic isotope effect (KIE) and kinetic energy release (KER) of protonated alkylamine dimers were studied by theor. modeling. In the calcns. on reaction kinetics one empirical parameter was used to describe the looseness of the transition state. Calcns. are compared to expts. described by Norrman and McMahon [Int. J. Mass. Spetrom. 182/183 (1999) 381]. In the case of expts. using a high-pressure ion source the Rice-Ramsperger-Kassel-Marcus (RRKM) model, taking into account energy distributions and the time scale of metastable ion fragmentation, accurately describes the exptl. obsd. KIE's of .alpha.-deuterated amines. The KER (available exptl. in one case only) is also correctly calcd., using no further parameters. In the case of low-pressure ion source, the internal energy **distribution** (IED) is not thermal, so it was empirically estd. based on the exptl. obsd. KIE. Using this est., it was possible to calc. the KER of .alpha.-deuterated amines accurately. Based on theor. expectations it was found that the mean KER value is equal to 3/2kTeff. This allows estn. of the KER in cases where it is detd. by statistical factors. Energy distributions of various fragmenting ion populations are discussed in some detail. These may be helpful for a qual. understanding of mass spectrometric processes and the theor. basis of the kinetic method.
REFERENCE COUNT: 56 THERE ARE 56 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 7 OF 87 MEDLINE on STN DUPLICATE 3
ACCESSION NUMBER: 2003324858 IN-PROCESS
DOCUMENT NUMBER: 22738469 PubMed ID: 12854652
TITLE: **QSPR**-based prediction of **adsorption** of halogenated aromatics on yellow-brown soil.
AUTHOR: Wei D B; Wu C D; Wang L S; Hu H Y
CORPORATE SOURCE: Department of Environmental Science and Engineering, ESPC State Key Joint Laboratory, Tsinghua University, Beijing 100084, People's Republic of China.. weidongbin@tsinghua.org.cn
SOURCE: SAR AND QSAR IN ENVIRONMENTAL RESEARCH, (2003 Jun) 14 (3) 191-8.
Journal code: 9440156. ISSN: 1062-936X.
PUB. COUNTRY: England: United Kingdom
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English
FILE SEGMENT: IN-PROCESS; NONINDEXED; Priority Journals
ENTRY DATE: Entered STN: 20030713
Last Updated on STN: 20030713
AB Halogenated aromatic compounds exist widely in soil and aqueous environment. The study of their transport and **distribution** is quite important for pollution control and risk assessment. In the present work the **adsorption** coefficients of 28 halogenated benzenes, anilines and phenols on yellow-brown soil were measured with batch equilibrium method, and a prediction model was developed through the

quantitative structure-property relationship (**QSPR**) technique. Then the obtained model was tested with Monte Carlo simulation and Jacknife methods. The results indicated that it was robust enough to estimate soil **adsorption** behaviors for the tested compounds. Based on the obtained model it could be deduced that the **adsorption** of halogenated aromatics on yellow-brown soil was not a simple partitioning process but involved complicated interactions.

L15 ANSWER 8 OF 87 MEDLINE on STN DUPLICATE 4
ACCESSION NUMBER: 2003389607 IN-PROCESS
DOCUMENT NUMBER: 22807538 PubMed ID: 12926856
TITLE: Predicting drug pharmacokinetic properties using molecular interaction fields and SIMCA.
AUTHOR: Wolohan Philippa R N; Clark Robert D
CORPORATE SOURCE: Tripos, Inc., 1699 South Hanley Road, Saint Louis, Missouri 63144, USA.. pwolohan@tripos.com
SOURCE: JOURNAL OF COMPUTER-AIDED MOLECULAR DESIGN, (2003 Jan) 17 (1) 65-76.
Journal code: 8710425. ISSN: 0920-654X.
PUB. COUNTRY: Netherlands
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English
FILE SEGMENT: IN-PROCESS; NONINDEXED; Priority Journals
ENTRY DATE: Entered STN: 20030821
Last Updated on STN: 20030821

AB We have developed a method that combines molecular interaction fields with soft independent modeling of class analogy (SIMCA) to predict pharmacokinetic drug properties. Several additional considerations to those made in traditional QSAR are required in order to develop a successful **QSPR** strategy that is capable of accommodating the many complex factors that contribute to key pharmacokinetic properties such as ADME (absorption, **distribution**, **metabolism**, and excretion) and toxicology. An accurate prediction of oral bioavailability, for example, requires that absorption and first-pass hepatic elimination both be taken into consideration. To accomplish this, general properties of molecules must be related to their solubility and ability to penetrate biological membranes, and specific features must be related to their particular metabolic and toxicological profiles. Here we describe a method, which is applicable to structurally diverse data sets while utilizing as much detailed structural information as possible. We address the issue of the molecular alignment of a structurally diverse set of compounds using idiotropic field orientation (IFO), a generalization of inertial field orientation. We have developed a second flavor of this method, which directly incorporates electrostatics into the molecular alignment. Both variations of IFO produce a characteristic orientation for each structure and the corresponding molecular fields can then be analyzed using SIMCA. Models are presented for human intestinal absorption, blood-brain barrier penetration and bioavailability to demonstrate ways in which this tool can be used early in the drug development process to identify leads likely to exhibit poor pharmacokinetic behavior in pre-clinical studies, and we have explored the influence of conformation and molecular field type on the statistical properties of the models obtained.

L15 ANSWER 9 OF 87 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2003:565108 CAPLUS
TITLE: **QSPR** study of imidazole and its derivatives as corrosion inhibitor of copper for hydrochloric acid pickling
AUTHOR(S): Zhao, Yong-sheng; Pang, Zheng-zhi; Lu, Yan-hua; Wang, Lei
CORPORATE SOURCE: College of Materials Science and Engineering, Beijing University of Chemical Technology, Beijing, 100029, Peop. Rep. China

SOURCE: Beijing Huagong Daxue Xuebao, Ziran Kexueban (2003), 30(3), 55-58
CODEN: BHDXAA; ISSN: 1671-4628
PUBLISHER: Beijing Huagong Daxue Xuebao, Ziran Kexueban Bianji Weiyuanhui
DOCUMENT TYPE: Journal
LANGUAGE: Chinese

AB The corrosion inhibition efficiencies of imidazole and its 12 derivs. for copper in 5% HCl soln. at 30 .degree.C were studied by a wt.-loss method. The main characteristic parameters of these compds. were obtained with a PM3 semiempirical quantum chem. block in hyperchem programs . The success and limitation of the quantum chem. method in this research were discussed, the relationship of the corrosion inhibition properties with the characteristic parameters was obtained by Quant. Structure-Property Relationship (**QSPR**), and the mechanism of corrosion inhibition of imidazole and its derivs. for copper were studied. The results indicate that the corrosion inhibition properties of imidazole and its derivs. have good correlations with the **distribution** coeffs., with the net charge of the imidazole rings and with the first order mol. connection indexes of the compds.

L15 ANSWER 10 OF 87 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2002:10123 CAPLUS
DOCUMENT NUMBER: 136:64091
TITLE: Method and system for predicting pharmacokinetic properties
INVENTOR(S): Hattori, Kazunari; Shimada, Kaore; Uchiyama, Mamoru
PATENT ASSIGNEE(S): Pfizer Inc., USA
SOURCE: Eur. Pat. Appl., 27 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1167969	A2	20020102	EP 2001-304648	20010525
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
US 2003069698	A1	20030410	US 2001-876767	20010607
JP 2003014728	A2	20030115	JP 2001-179774	20010614

PRIORITY APPLN. INFO.: US 2000-211864P P 20000614

AB This invention provides a method for predicting pharmacokinetic properties of mols. comprising the steps of: (a) prepg. 2D-structures of mols. used as a training set; (b) constructing a 2D-fingerprint by counting the no. of structural descriptors that potentially relate to a pharmacokinetic property, either manually or automatically using internally developed macro; wherein said structural descriptors consist of predefined 20 to 80 atoms/fragments or substructures; (c) analyzing the obtained 2D-fingerprint by a statistical anal. method to correlate with the pharmacokinetic property of the mol. to yield a quant. structure-property relation (**QSPR**) model; and (d) calcg. the pharmacokinetic property of a trial mol. using the above obtained **QSPR** model. A system for this invention is also provided. According to this method and system, it is possible to predict pharmacokinetic properties of mols. prior to synthesis, without labor-intensive and time-consuming experimentation.

L15 ANSWER 11 OF 87 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2002:509499 CAPLUS
DOCUMENT NUMBER: 137:194997
TITLE: Descriptors, physical properties, and drug-likeness
AUTHOR(S): Bruestle, Matthias; Beck, Bernd; Schindler, Torsten;

King, William; Mitchell, Timothy; Clark, Timothy
CORPORATE SOURCE: Computer-Chemie-Centrum, Friedrich-Alexander-Universitaet Erlangen-Nuernberg, Erlangen, D-91052, Germany
SOURCE: Journal of Medicinal Chemistry (2002), 45(16), 3345-3355
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB We have investigated techniques for distinguishing between drugs and nondrugs using a set of mol. descriptors derived from semiempirical MO (AM1) calcns. The "drug" data set of 2105 compds. was derived from the World Drug Index (WDI) using a procedure designed to select real drugs. The "nondrug" data set was the Maybridge database. We have first investigated the dimensionality of phys. properties space based on a set of 26 descriptors that we have used successfully to build absorption, **distribution**, metab., and excretion-related quant. structure-property relationship models. We discuss the general nature of the descriptors for phys. property space and the ability of these descriptors to distinguish between drugs and nondrugs. The third most significant principal component of this set of descriptors serves as a useful numerical index of drug-likeness, but no others are able to distinguish between drugs and nondrugs. We have therefore extended our set of descriptors to a total of 66 and have used recursive partitioning to identify the descriptors that can distinguish between drugs and nondrugs. This procedure pointed to two of the descriptors that play an important role in the principal component found above and one more from the set of 40 extra descriptors. These three descriptors were then used to train a Kohonen artificial neural net for the entire Maybridge data set. Projecting the drug database onto the map obtained resulted in a clear distinction not only between drugs and nondrugs but also, for instance, between hormones and other drugs. Projection of 42 131 compds. from the WDI onto the Kohonen map also revealed pronounced clustering in the regions of the map assigned as druglike.

REFERENCE COUNT: 49 THERE ARE 49 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 12 OF 87 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2002:821535 CAPLUS
DOCUMENT NUMBER: 138:141359
TITLE: Estimation of activated carbon **adsorption** efficiency for organic vapours. I. A strategy for selecting test compounds
AUTHOR(S): Fangmark, Ingrid E.; Hammarstrom, Lars-Gunnar; Stromqvist, Marianne E.; Ness, Amanda L.; Norman, Paul R.; Osmond, Neale M.
CORPORATE SOURCE: Swedish Defence Research Agency, FOI, Umea, SE-901 82, Swed.
SOURCE: Carbon (2002), 40(15), 2861-2869
CODEN: CRBNAH; ISSN: 0008-6223
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Strategies for developing quant. structure-affinity relationships (QSAfR) for the prediction of break-through performance of 31 chlorinated hydrocarbons on activated carbon have been studied. Two different approaches for the selection of a limited set of compds. for modeling were evaluated through the predictive power of the resulting QSAfR models. When the model was based on a training-set selected without a rational strategy, the developed QSAfR model showed poor predictive performance. Accordingly, such models have a limited capability to produce information concerning the important adsorbate related parameters influencing **adsorption**. By using a strategy where multivariate data anal.

techniques are used in conjunction with statistical exptl. design to select a balanced set of compds. for break-through performance evaluation, it was possible to develop QSAfR models with high predictive capability.
REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 13 OF 87 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2002:629041 CAPLUS
DOCUMENT NUMBER: 137:352669
TITLE: Vapor pressures, aqueous solubilities, and Henry's law constants of some brominated flame retardants
AUTHOR(S): Tittlemier, Sheryl A.; Halldorson, Thor; Stern, Gary A.; Tomy, Gregg T.
CORPORATE SOURCE: Centre for Analytical and Environmental Chemistry, Carleton University, Ottawa, ON, K1S 5B6, Can.
SOURCE: Environmental Toxicology and Chemistry (2002), 21(9), 1804-1810
CODEN: ETOCDK; ISSN: 0730-7268
PUBLISHER: SETAC Press
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The subcooled liq. vapor pressures (PL.250s) and aq. solubilities (SW.25s) were detd. and Henry's law consts. (H25s) were estd. for a no. of brominated flame retardants (BFRs) at 25.degree.. The established methods of the gas chromatog.-retention time and generator column techniques were used to exptl. det. PL.250 and SW.25 for hexabromobenzene and brominated di-Ph ether (BDE) congeners. The H25 was estd. as the ratio of PL.250 to the subcooled liq. aq. soly. Values of PL.250 obtained ranged from 0.000000282 Pa (BDE-190) to 0.259 Pa (BDE-3); SW.25 ranged from 0.00000087 g/L (BDE-153 and BDE-154) to 0.00013 g/L (BDE-15); and H25 ranged from 0.0074 Pa m3/mol (BDE-183) to 21 Pa m3/mol (BDE-15). An increase in the Br content of polybrominated di-Ph ether congeners resulted in significant decreases of PL.250, SW.25, and H25. A simple four-compartment equil. **distribution** model suggested that the majority of BFRs being released into the environment would reside in soil and sediment and have localized distributions. The model also suggested that lower brominated congeners tend to be somewhat more mobile. Degradative debromination reactions that yield these congeners would mobilize them environmentally, and ultimately affect the fate and **distribution** of BFRs.
REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 14 OF 87 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2002:697686 CAPLUS
DOCUMENT NUMBER: 138:358281
TITLE: Structure-property relationships of thioacridines; their electrochemical oxidation as a model of metabolic degradation
AUTHOR(S): Nesmerak, K.; Nemec, I.; Sticha, M.; Nemcova, I.; Horka, V.
CORPORATE SOURCE: Departments of Analytical Chemistry, Charles University of Prague, Prague, 128 43/2, Czech Rep.
SOURCE: Analytical Letters (2002), 35(10), 1617-1629
CODEN: ANALBP; ISSN: 0003-2719
PUBLISHER: Marcel Dekker, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The relationships of structure vs. electrochem. and vs. chromatog. properties of thirteen 9-(alkylthio)acridines were studied and quantified by correlation equations between E1/2 (tr, resp.), and substituent consts. The study of electrochem. oxidn. of these compds. as the model of their possible metabolic degrdn. was performed. The oxidn. products were sepd. and analyzed by mass spectrometry. The probable scheme of electrochem. oxidn. of studied derivs. was proposed.

REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 15 OF 87 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2002:741098 CAPLUS
DOCUMENT NUMBER: 137:384463
TITLE: A Comparison between the Two General Sets of Linear Free Energy Descriptors of Abraham and Klamt
AUTHOR(S): Zissimos, Andreas M.; Abraham, Michael H.; Klamt, Andreas; Eckert, Frank; Wood, John
CORPORATE SOURCE: Department of Chemistry, University College London, London, WC1H OAJ, UK
SOURCE: Journal of Chemical Information and Computer Sciences (2002), 42(6), 1320-1331
CODEN: JCISD8; ISSN: 0095-2338
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Two sets of mol. descriptors, the five exptl. Abraham, and the five COSMOments of Klamt's COSMO-RS, have been compared for a data set of 470 compds. Both sets are considered as almost complete sets of LFER. The two sets of descriptors are shown to exhibit a large overlap as far as their chem. content. The chem. information however is distributed differently in each set with the Abraham set incorporating extra information in the excess molar refraction descriptor E. Regression equations have been constructed to predict the exptl. Abraham descriptors from theor. calcd. COSMOments. The chem. interpretation of these equations is however difficult because of the lack of clustering which characterizes the **distribution** of chem. information through the two sets of descriptors. The predictability of the regression equations is tested successfully using a reasonably large set of data, and the method is compared to recent attempts to calc. the Abraham descriptors from various theor. bases.
REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 16 OF 87 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2002:360438 CAPLUS
DOCUMENT NUMBER: 137:63008
TITLE: Improving the Predicting Power of Partial Order Based QSARs through Linear Extensions
AUTHOR(S): Carlsen, Lars; Lerche, Dorte B.; Sorensen, Peter B.
CORPORATE SOURCE: Department of Environment Technology and Social Studies, Roskilde University, Roskilde, DK-4000, Den.
SOURCE: Journal of Chemical Information and Computer Sciences (2002), 42(4), 806-811
CODEN: JCISD8; ISSN: 0095-2338
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Partial order theory (POT) is an attractive and operationally simple method that allows ordering of compds., based on selected structural and/or electronic descriptors (modeled order), or based on their end points, e.g., soly. (exptl. order). If the modeled order resembles the exptl. order, compds. that are not exptl. investigated can be assigned a position in the model that eventually might lead to a prediction of an end-point value. However, in the application of POT in quant. structure-activity relationship modeling, only the compds. directly comparable to the noninvestigated compds. are applied. To explore the possibilities of improving the methodol., the theory is extended by application of the so-called linear extensions of the model order. The study show that partial ordering combined with linear extensions appears as a promising tool providing probability **distribution** curves in the range of possible end-point values for compds. not being exptl.

investigated.
REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 17 OF 87 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2002:915740 CAPLUS
DOCUMENT NUMBER: 138:187239
TITLE: Multivariate characterization of polycyclic aromatic hydrocarbons using semi-empirical molecule orbital calculations and physical data
AUTHOR(S): Kitti, Anna; Harju, Mikael; Tysklind, Mats; van Bavel, Bert
CORPORATE SOURCE: Environmental Chemistry, Umea University, Umea, 901 87, Swed.
SOURCE: Chemosphere (2002), Volume Date 2003, 50(5), 627-637
CODEN: CMSHAF; ISSN: 0045-6535
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Multivariate characterization of 60 polycyclic arom. hydrocarbons (PAHs) was performed using data from literature and semi-empirical MO calcns. This dataset was analyzed by principal component anal. and projections to latent structures by partial least square. The PAHs distribute in the chem. domain in several groups mainly governed by the no. of arom. rings and the no. of five-membered rings. The multivariate model and training set was used to predict GC retention times on a nonpolar column (DB-5). Using a 24 exptl. design on the principal components of the chem. characterization model, a test set of PAHs was selected dependent on the **distribution** in the chem. domain of the PAHs. Such a test set is expected to improve selection of PAHs for future testing and modeling of both biol. and chem. responses. Although the model of GC retention times was good, the precision was however not good enough for practical use.
REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 18 OF 87 BIOSIS COPYRIGHT 2003 BIOLOGICAL ABSTRACTS INC. on STN
DUPLICATE 5
ACCESSION NUMBER: 2002:570571 BIOSIS
DOCUMENT NUMBER: PREV200200570571
TITLE: Computer-aided drug design: The role of quantitative structure-property, structure-activity and structure-**metabolism** relationships (**QSPR**, QSAR, QSMR.
AUTHOR(S): Buchwald, Peter; Bodor, Nicholas (1)
CORPORATE SOURCE: (1) IVAX Research, Inc., 4400 Biscayne Boulevard, Miami, FL, 33137 USA
SOURCE: Drugs of the Future, (June, 2002) Vol. 27, No. 6, pp. 577-588. print.
ISSN: 0377-8282.
DOCUMENT TYPE: General Review
LANGUAGE: English

L15 ANSWER 19 OF 87 MEDLINE on STN DUPLICATE 6
ACCESSION NUMBER: 2003008866 MEDLINE
DOCUMENT NUMBER: 22403089 PubMed ID: 12515349
TITLE: Prediction of vapour pressures for halogenated diphenyl ether congeners from molecular descriptors.
AUTHOR: Oberg Tomas G
CORPORATE SOURCE: T. Oberg Konsult AB, Gamla Brov. 13, SE-371 60 Lyckeby, Sweden.. info@tomasoberg.com
SOURCE: Environ Sci Pollut Res Int, (2002) 9 (6) 405-11.
Journal code: 9441769. ISSN: 0944-1344.
PUB. COUNTRY: Germany: Germany, Federal Republic of
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)

LANGUAGE: English
FILE SEGMENT: Priority Journals
ENTRY MONTH: 200301
ENTRY DATE: Entered STN: 20030108
Last Updated on STN: 20030129
Entered Medline: 20030128

AB BACKGROUND, AIM AND SCOPE: Polychlorinated diphenyl ethers (PCDE) and polybrominated diphenyl ethers (PBDE) have both been identified as environmental contaminants. The physical properties are important in determining the **distribution** and fate of organic contaminants in the environment. The purpose of the present investigation was to characterise halogenated diphenyl ethers using computationally derived descriptors, and to develop calibration models for the vapour pressure from published experimental data. METHODS: Experimental data for vapour pressures were obtained from the literature. The chemical structure of each PCDE and PBDE congener was optimised prior to descriptor generation. The data analysis was performed using principal component analysis (PCA) and partial least squares regression (PLSR). The calibration models were validated with external test sets. RESULTS AND DISCUSSION: All congeners of PCDEs and PBDEs were characterised by 795 molecular descriptors and two principal components could account for about two thirds of the variance within each group. Bilinear calibration models were developed that could explain 99.4% of the variance in the external validation test sets. Vapour pressures were subsequently predicted for all congeners that were adequately described by these calibration models. The type and number of halogen atoms in the molecule were the main factors influencing the vapour pressures of halogen substituted diphenyl ethers, but the variations in substitution pattern was also shown to be a significant factor. CONCLUSIONS: The molecular descriptor patterns of halogenated aromatic compounds such as diphenyl ethers can be described and interpreted using principal component analysis (PCA). The major sources of variation in the descriptor spaces for PCDEs and PBDEs are the same as those contributing to the differences in vapour pressure, similar to what has previously been reported for the PCBs. The bilinear calibration models for vapour pressure presented here, has a standard error of prediction that is lower than what is reported as the experimental uncertainty or observed as deviations between experimental investigations. The estimated prediction errors are expected to be within the reported boundaries when the models are applied to new objects within the same molecular descriptor space, and model predictions can hence extend the current database of experimental values. RECOMMENDATIONS AND OUTLOOK: The results from this investigation and others show that the establishment of quantitative structure-property relationships (**QSPR**) is a viable approach to estimate physical properties for halogenated diphenyl ethers. It is easy to foresee an increased need for using **QSPR** estimation methods in the future, for evaluation of the environmental fate for organic pollutants. Despite method developments and automation, it is unlikely that laboratory determinations can cope with the pace that new pollutants are identified.

L15 ANSWER 20 OF 87 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2002:567583 CAPLUS
DOCUMENT NUMBER: 137:299216
TITLE: Use of QSPRS in improving carbon **adsorption** modeling of EPA contaminant candidate compounds
AUTHOR(S): Magnuson, Matthew L.; Speth, Thomas F.
CORPORATE SOURCE: Office of Research and Development, National Risk Management Research Laboratory, Water Supply and Water Resources Division, US Environmental Protection Agency, Cincinnati, OH, 45268, USA
SOURCE: Preprints of Extended Abstracts presented at the ACS National Meeting, American Chemical Society, Division of Environmental Chemistry (2002), 42(2), 366-369
CODEN: PEACF2; ISSN: 1524-6434
PUBLISHER: American Chemical Society, Division of Environmental

Chemistry
DOCUMENT TYPE: Journal; (computer optical disk)
LANGUAGE: English
AB A more accurate means to assess the cost of using activated carbon to treat water contaminated with a particular EPA contaminant candidate compd. can be obtained by employing the quant. structure property relations (**QSPR**) approach, which reconciles the differences between two carbon **adsorption** models. Through the correct selection of descriptors, the carbon use rates calcd. using **QSPR** -enhanced Model 1 agree better with those calcd. using Model 2. The better agreement, from an engineering design standpoint, increases confidence in both models. This may ultimately translate into accurate cost predictions for use in upcoming regulations.
REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> s l11 not py<2000
2 FILES SEARCHED...
L16 88 L11 NOT PY<2000

=> s l15 not py<2000
2 FILES SEARCHED...
L17 63 L15 NOT PY<2000

=> d ibib abs l17 1

L17 ANSWER 1 OF 63 MEDLINE on STN
ACCESSION NUMBER: 2003389607 IN-PROCESS
DOCUMENT NUMBER: 22807538 PubMed ID: 12926856
TITLE: Predicting drug pharmacokinetic properties using molecular interaction fields and SIMCA.
AUTHOR: Wolohan Philippa R N; Clark Robert D
CORPORATE SOURCE: Tripos, Inc., 1699 South Hanley Road, Saint Louis, Missouri 63144, USA.. pwolohan@tripos.com
SOURCE: JOURNAL OF COMPUTER-AIDED MOLECULAR DESIGN, (2003 Jan) 17 (1) 65-76.
Journal code: 8710425. ISSN: 0920-654X.
PUB. COUNTRY: Netherlands
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English
FILE SEGMENT: IN-PROCESS; NONINDEXED; Priority Journals
ENTRY DATE: Entered STN: 20030821
Last Updated on STN: 20030821
AB We have developed a method that combines molecular interaction fields with soft independent modeling of class analogy (SIMCA) to predict pharmacokinetic drug properties. Several additional considerations to those made in traditional QSAR are required in order to develop a successful **QSPR** strategy that is capable of accommodating the many complex factors that contribute to key pharmacokinetic properties such as ADME (absorption, **distribution**, **metabolism**, and excretion) and toxicology. An accurate prediction of oral bioavailability, for example, requires that absorption and first-pass hepatic elimination both be taken into consideration. To accomplish this, general properties of molecules must be related to their solubility and ability to penetrate biological membranes, and specific features must be related to their particular metabolic and toxicological profiles. Here we describe a method, which is applicable to structurally diverse data sets while utilizing as much detailed structural information as possible. We address the issue of the molecular alignment of a structurally diverse set of compounds using idiotropic field orientation (IFO), a generalization of inertial field orientation. We have developed a second flavor of this method, which directly incorporates electrostatics into the molecular alignment. Both variations of IFO produce a characteristic orientation

for each structure and the corresponding molecular fields can then be analyzed using SIMCA. Models are presented for human intestinal absorption, blood-brain barrier penetration and bioavailability to demonstrate ways in which this tool can be used early in the drug development process to identify leads likely to exhibit poor pharmacokinetic behavior in pre-clinical studies, and we have explored the influence of conformation and molecular field type on the statistical properties of the models obtained.

=> d his

(FILE 'HOME' ENTERED AT 16:27:17 ON 29 SEP 2003)

FILE 'MEDLINE, BIOSIS, BIOTECHDS, CAPLUS, EMBASE' ENTERED AT 16:27:32 ON 29 SEP 2003

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L1          1391 S QSPR
L2            14 S 2D FINGERPRINT
L3             2 S L1 AND L2
L4           189 S 2D STRUCTURE
L5             0 S L1 AND L4
L6        142325 S PHARMACOKINETIC
L7             0 S L4 AND L6
L8           649 S ADME
L9             1 S L4 AND L8
L10      6895655 S ADSORPTION OR DISTRIBUTION OR METABOLISM OR EXRETION
L11          119 S L1 AND L10
L12           28 S L4 AND L10
L13           46 S L11 NOT PY>2000
L14           37 DUP REM L13 (9 DUPLICATES REMOVED)
L15           87 DUP REM L11 (32 DUPLICATES REMOVED)
L16           88 S L11 NOT PY<2000
L17           63 S L15 NOT PY<2000
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=> d ibib abs l14 1

L14 ANSWER 1 OF 37 CAPLUS COPYRIGHT 2003 ACS on STN

```
ACCESSION NUMBER:         2000:537854  CAPLUS
DOCUMENT NUMBER:          133:222218
TITLE:                    Stability of Complexes of Aromatic Amides with Bromide
                          Anion: Quantitative Structure-Property Relationships
AUTHOR(S):                Cajan, Michal; Damborsky, Jiri; Stibor, Ivan; Koca,
                          Jaroslav
CORPORATE SOURCE:         Laboratory of Biomolecular Structure and Dynamics and
                          Department of Organic Chemistry Faculty of Science,
                          Masaryk University, Brno, 611 37, Czech Rep.
SOURCE:                   Journal of Chemical Information and Computer Sciences
                          (2000), 40(5), 1151-1157
                          CODEN: JCISD8; ISSN: 0095-2338
PUBLISHER:                American Chemical Society
DOCUMENT TYPE:            Journal
LANGUAGE:                 English
```

AB Most of the theor. studies published to-date on the structural and electronic properties of supramols. have been devoted to the neutral or cationic complexes, while little is known about anionic systems. A detailed theor. study of the interaction between simple arom. amides and the bromide anion has recently been published (Cajan, M.; Stibor, I.; Koca, J. J. Phys. Chem. A 1999, 103, 3778). The present work focuses on the structural and physicochem. parameters of simple arom. amides related to their ability to form the 1:1 complex with a bromide anion. A quant. structure-property relationships (**QSPR**) model for the prediction of assocn. consts. is proposed. The model based on 22 complexes and nine mol. descriptors explained 96% (84% cross-validated) of the variance in assocn. consts. The descriptors employed in this model included

parameters for the characterization of conformational behavior and the 3D structure of amide mols., **distribution** of electron d. on the amidic functional group, and parameters for substitution on arom. units. The quant. structure-property relationship approach predicted the assocn. consts. with comparable quality, but significantly lower computational demand, than mol. modeling or std. quantum chem. calcns.
REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d ibib abs l14 1-37

L14 ANSWER 1 OF 37 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2000:537854 CAPLUS
DOCUMENT NUMBER: 133:222218
TITLE: Stability of Complexes of Aromatic Amides with Bromide Anion: Quantitative Structure-Property Relationships
AUTHOR(S): Cajan, Michal; Damborsky, Jiri; Stibor, Ivan; Koca, Jaroslav
CORPORATE SOURCE: Laboratory of Biomolecular Structure and Dynamics and Department of Organic Chemistry Faculty of Science, Masaryk University, Brno, 611 37, Czech Rep.
SOURCE: Journal of Chemical Information and Computer Sciences (2000), 40(5), 1151-1157
CODEN: JCISD8; ISSN: 0095-2338
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Most of the theor. studies published to-date on the structural and electronic properties of supramols. have been devoted to the neutral or cationic complexes, while little is known about anionic systems. A detailed theor. study of the interaction between simple arom. amides and the bromide anion has recently been published (Cajan, M.; Stibor, I.; Koca, J. J. Phys. Chem. A 1999, 103, 3778). The present work focuses on the structural and physicochem. parameters of simple arom. amides related to their ability to form the 1:1 complex with a bromide anion. A quant. structure-property relationships (**QSPR**) model for the prediction of assocn. consts. is proposed. The model based on 22 complexes and nine mol. descriptors explained 96% (84% cross-validated) of the variance in assocn. consts. The descriptors employed in this model included parameters for the characterization of conformational behavior and the 3D structure of amide mols., **distribution** of electron d. on the amidic functional group, and parameters for substitution on arom. units. The quant. structure-property relationship approach predicted the assocn. consts. with comparable quality, but significantly lower computational demand, than mol. modeling or std. quantum chem. calcns.
REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 2 OF 37 MEDLINE on STN
ACCESSION NUMBER: 2001019812 MEDLINE
DOCUMENT NUMBER: 20320152 PubMed ID: 10864156
TITLE: Electronic eigenvalue (EEVA): a new QSAR/**QSPR** descriptor for electronic substituent effects based on molecular orbital energies. A QSAR approach to the Ah receptor binding affinity of polychlorinated biphenyls (PCBs), dibenzo-p-dioxins (PCDDs) and dibenzofurans (PCDFs).
AUTHOR: Tuppurainen K; Ruuskanen J
CORPORATE SOURCE: Department of Chemistry, University of Kuopio, Finland.. kari.tuppurainen@uku.fi
SOURCE: CHEMOSPHERE, (2000 Sep) 41 (6) 843-8.
Journal code: 0320657. ISSN: 0045-6535.
PUB. COUNTRY: ENGLAND: United Kingdom

DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English
FILE SEGMENT: Priority Journals
ENTRY MONTH: 200011
ENTRY DATE: Entered STN: 20010322
Last Updated on STN: 20010322
Entered Medline: 20001103

AB A new descriptor of molecular structure for use in the derivation of predictive QSAR and **QSPR** models, electronic eigenvalue (EEVA), is described. This is a modification of the recently proposed EVA approach, but is based on computationally-derived molecular orbital energies instead of vibrational frequencies. Like EVA, it is also invariant as to the alignment of the structures concerned. Its performance has been tested with respect to the Ah receptor binding of PCBs, PCDDs and PCDFs, and its predictive ability has been clearly demonstrated. In particular, it seems to be suitable for 'pure' electronic substituent effects. i.e., for cases in which both hydrophobic and steric factors are of minor importance.

L14 ANSWER 3 OF 37 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2000:201651 CAPLUS
DOCUMENT NUMBER: 132:308036
TITLE: Estimation of hydrophobicity using quasi-molecular volume of quarternary ammonium ions
AUTHOR(S): Ohtsuka, Chizuko; Mori, Yasuyuki; Hayashi, Shigeyuki; Tsuda, Takao; Wada, Hiroko
CORPORATE SOURCE: Aichi Mizuho College, Nagoya, Japan
SOURCE: Journal of Liquid Chromatography & Related Technologies (2000), 23(5), 669-680
CODEN: JLCTFC; ISSN: 1082-6076
PUBLISHER: Marcel Dekker, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB When the Cu(II), Co(III), Ni(II), and Fe(II) chelates with 2-(5-Nitro-2-pyridyl)-5-[N-propyl-N-(sulfopropyl)amino]phenol (Nitro-PAPS) were sepd. on octadecylsilane (ODS) stationary phase (Kaseisorb ODS Super and Kaseisorb LC ODS-300-5) by the addn. of several quaternary ammonium salts (Q+Br) individually to the aq. ACN mobile phase, a correlation of these hydrophobic cation's character with the retention of the chelates was examd. The degree of the variation of the stationary phase due to the **adsorption** of quaternary ammonium ion (Q+) is measured by using elution time of a solute, which were obtained by its successive injection. When the alkyl group of Q+ is larger, the period for attaining the equil. becomes longer. As a concn. of Q+ is higher, the period becomes longer. The estn. of quasi-mol. vol. is proposed. The estn. vol. provides its 1st order relation with log k' of the metal chelates, regardless of the difference of its charged position in the structure. The degree of the slope of the 1st order relation corresponds to the no. of Q+ assocd. with metal/Nitro-PAPS chelate. The elution order corresponds to the total no. of Q+ and Nitro-PAPS being assocd. with metal ions.

REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 4 OF 37 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2000:608078 CAPLUS
DOCUMENT NUMBER: 133:168050
TITLE: Sorption study of substituted aromatic ketone in soil by batch equilibrium method
AUTHOR(S): Ding, Yanbin; Song, Weihua; Wang, Liansheng
CORPORATE SOURCE: State Key Laboratory of Pollution Control and Resource Reuse, School of Environment, Nanjing University, Nanjing, 210093, Peop. Rep. China
SOURCE: Huanjing Huaxue (2000), 19(4), 330-334
CODEN: HUHUDB; ISSN: 0254-6108

PUBLISHER: Kexue Chubanshe
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
AB The sorption of 12 substituted arom. ketone compds. by black soil from northeastern China was studied using batch equil. method. The data were fitted to the Freundlich equation with the regression anal. The results showed that the sorption behaviors of 12 substituted arom. ketone compds. could be characterized by linear and non-linear isotherms suggesting different sorption mechanisms. A **QSPR** equation was established and indicated that mol. polarity was an potential factor affecting the org. carbon sorption coeffs. of these 12 substituted arom. ketones in soils.

L14 ANSWER 5 OF 37 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2000:221793 CAPLUS
DOCUMENT NUMBER: 132:242263
TITLE: **QSPR** of interfacial phenomena of 8-sulfonamidoquinolines
AUTHOR(S): Sakoguchi, Akihiro; Zushi, Eita; Ueoka, Ryuichi; Nakashio, Fumiyuki; Yoshizuka, Kazuharu
CORPORATE SOURCE: Department of Applied Chemistry, Kumamoto Institute of Technology, Kumamoto, 860-0082, Japan
SOURCE: Kagaku Kogaku Ronbunshu (2000), 26(2), 305-308
CODEN: KKRBAW; ISSN: 0386-216X
PUBLISHER: Kagaku Kogakkai
DOCUMENT TYPE: Journal
LANGUAGE: Japanese
AB To realize quant. elucidation, as well as simulate complex formation at the liq.-liq. interface, 8-sulfonamidoquinolines (CnphSAQ) were calcd. by both a semi-empirical MO method considering solvent effect, and mol. dynamics at the H2O-toluene interface. The MD calcns. support the fact that interfacial area occupied by a mol. (.apprx.60 .ANG.2) obtained by the measurement of interfacial equil. of CnphSAQ is consistent with projected area of sulfonamidoquinoline moiety. Also, examn. of the quant. structure property relation (**QSPR**) between energy difference in interfacial **adsorption** and interfacial **adsorption** equil. const. can obtain good linear correlation.

L14 ANSWER 6 OF 37 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2000:677838 CAPLUS
DOCUMENT NUMBER: 133:227358
TITLE: Prediction of partition properties of substituted benzaldehydes using different structural parameters
AUTHOR(S): Dai, Jia-Yin; Han, Shuo-Kui; Wang, Lian-Sheng
CORPORATE SOURCE: State Key Laboratory of Pollution Control and Resource Reuse, Tongji University, Shanghai, 200092, Peop. Rep. China
SOURCE: Zhongguo Huanjing Kexue (2000), 20(4), 292-295
CODEN: ZHKEEI; ISSN: 1000-6923
PUBLISHER: Zhongguo Huanjing Kexue Bianji Weiyuanhui
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
AB The octanol/water partition coeffs. (Kow) and water soly. (Sw) for 28 substituted benzaldehydes were detd. Quantum chem. parameters and mol. connectivity indexes were used to develop quant. structure-property relationships (**QSPR**) models. The models could predict effectively the Kow and Sw of the tested compds. The mean residuals of the estd. Kow and Sw of the compds. were 0.15, 0.20 log units resp. Results demonstrated that the independent variables in the models did not interrelate mutually; and the residuals presented normal **distribution**.

L14 ANSWER 7 OF 37 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2000:882982 CAPLUS

DOCUMENT NUMBER: 134:360969
TITLE: **QSPR** prediction of Henry's law constant: improved correlation with new parameters
AUTHOR(S): Dearden, John C.; Ahmed, Shazia A.; Cronin, Mark T. D.; Sharra, Janeth A.
CORPORATE SOURCE: School of Pharmacy and Chemistry, Liverpool John Moores University, Liverpool, L3 3AF, UK
SOURCE: Molecular Modeling and Prediction of Bioactivity, [Proceedings of the European Symposium on Quantitative Structure-Activity Relationships: Molecular Modeling and Prediction of Bioactivity], 12th, Copenhagen, Denmark, Aug. 23-28, 1998 (2000), Meeting Date 1998, 273-274. Editor(s): Gundertofte, Klaus; Jorgensen, Flemming Steen. Kluwer Academic/Plenum Publishers: New York, N. Y.
CODEN: 69ASO3
DOCUMENT TYPE: Conference
LANGUAGE: English
AB Henry's law const. (H) is the air-water partition coeff., and as such is important in modeling the environmental **distribution** of chems. Several quant. structure-property relation (**QSPR**) studies have been made of Henry's law const. Such a **QSPR** has been recently developed from a consideration of the fundamental processes occurring during air-water partitioning, and using only calcd. parameters. The equation developed, while giving reasonable predictions, has a rather high std. error, and the present study has been directed towards reducing this. New quant. hydrogen bonding parameters including a parameter that reflects conformational entropy change, were used. There was considerable improvement in the equation, esp. with regard to the std. error. Using a test set of 48 different compds., the modified equation gave a good correlation between the obsd. and predicted log H values.
REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 8 OF 37 MEDLINE on STN
ACCESSION NUMBER: 2001090291 MEDLINE
DOCUMENT NUMBER: 20419337 PubMed ID: 10966153
TITLE: Structure-property relationships on histamine H3-antagonists: binding of phenyl-substituted alkylthioimidazole derivatives to rat plasma proteins.
AUTHOR: Silva C; Plazzi P V; Bordi F; Rivara S; Vacondio F; Zuliani V; Caretta A; Mor M
CORPORATE SOURCE: Dipartimento Farmaceutico, Universita degli Studi di Parma, Viale delle Scienze, Italy.
SOURCE: FARMACO, (2000 Apr) 55 (4) 239-45.
Journal code: 8912641. ISSN: 0014-827X.
PUB. COUNTRY: Italy
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English
FILE SEGMENT: Priority Journals
ENTRY MONTH: 200101
ENTRY DATE: Entered STN: 20010322
Last Updated on STN: 20010322
Entered Medline: 20010125
AB The binding of a series of H3-antagonists to rat plasma proteins was investigated by dialysis experiments, with RP-HPLC measurement of the free ligand. The series was composed of 4(5)-phenyl-2-[[2-[4(5)-imidazolyl]ethyl]thio]imidazoles having, on the phenyl ring, meta- and para-substituents, with different physico-chemical characteristics. As high protein binding had been proposed as being one of the features limiting brain access for the reference H3-antagonist thioperamide, the title series was employed to test the possibility of achieving lower protein binding by modulation of lipophilicity, while maintaining good receptor affinity. The compounds tested showed quotas of bound drug

ranging from 60 to 97.5%, while for thioperamide a 78% bound drug quota was observed at high total concentrations, with a steep increase in bound percentage at lower concentrations. Two of the tested compounds, having a carboxamide substituent, showed lower protein binding compared to thioperamide over a wide range of total concentration, without a significant loss in affinity with respect to the parent compound. A strict dependence of protein binding on lipophilicity was observed, and a **QSPR** model was derived which could also account for the protein binding observed for thioperamide, while receptor affinity had been reported to be quite insensitive to phenyl ring substitution. It is therefore possible to modulate protein binding of these H3-antagonists, through lipophilicity adjustment, without losing receptor affinity; this finding could help in the design of new compounds with improved brain access.

L14 ANSWER 9 OF 37 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2000:794648 CAPLUS
TITLE: Numerical drug-fitness index.
AUTHOR(S): Clark, Tim
CORPORATE SOURCE: Friedrich-Alexander-Universitat Erlangen-Nurnberg, D-91052 Erlangen, N/A, Germany
SOURCE: Abstracts of Papers - American Chemical Society (2000), 220th, COMP-136
CODEN: ACSRAL; ISSN: 0065-7727
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal; Meeting Abstract
LANGUAGE: English

AB Recently, the emphasis in computational drug design has been shifting from the traditional quant. structuree-activity raletaionship (QSAR) techniques used to find biol. active mols. to more quant. structure-property relationship (**QSPR**-) oriented ests. of the absorption, **distribution**, metab., excretion (ADME) properties of mols. As part of this shift in emphasis, several groups have attempted to define the "drug-likedness" of mols. following the pioneering "rule of five" work by Lipinski. The most common approach to this problem has been to use some type of mol. descriptors linked with a patter recognition or interpolation technique, such as neural nets, in order to distinguish between a dataset of drugs and one of non-drugs. The main difficulty lies in the definition of non-drugs. Most chem. databases contain a very significant proprtion of mols. that would make good drugs if they were biol. active. A clear distiction between drugs and non-drugs can therefore be very difficult. An alternative approach, on which for instance the rule of five is based, is to use only drugs to set up a phys. property profile, rather than to look for distinctions between drugs and non-drugs. We now report a technique of this type designed to assign a numerical value to the "drug likedness" of a mol. We call this numerical value the "drug fitness" in the following in order to distinguish it from other measures of drug-likedness.

L14 ANSWER 10 OF 37 MEDLINE on STN
ACCESSION NUMBER: 2000121094 MEDLINE
DOCUMENT NUMBER: 20121094 PubMed ID: 10655641
TITLE: **QSPR** correlation and predictions of GC retention indexes for methyl-branched hydrocarbons produced by insects.
AUTHOR: Katritzky A R; Chen K; Maran U; Carlson D A
CORPORATE SOURCE: Department of Chemistry, University of Florida, Gainesville 32611-7200, USA.. katritzky@chem.ufl.edu
SOURCE: ANALYTICAL CHEMISTRY, (2000 Jan 1) 72 (1) 101-9.
Journal code: 0370536. ISSN: 0003-2700.
PUB. COUNTRY: United States
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English
FILE SEGMENT: Priority Journals

ENTRY MONTH: 200004
ENTRY DATE: Entered STN: 20000413
Last Updated on STN: 20000413
Entered Medline: 20000404

AB A successful interpretation of the complex manner by which the GC retention indexes of methylalkanes produced by insects are related to chemical structure was achieved using the quantitative structure-property relationship (**QSPR**) method. A general **QSPR** model including mainly topological descriptors was obtained for 178 data points. The error of the model is similar to the experimental error. The model was supported by (i) leave-one-out cross validation and (ii) division into three sets and prediction of each set from the other two. As a further test of the utility of the model, retention indexes were successfully predicted for an external set of 30 methyl-branched hydrocarbons not involved in the deduction of the correction equation from the main data set. General trends of the structural variation of compounds in any given range of retention index are discussed. The average error was 4.6 overall and 4.3 for the 165 compounds remaining after leaving out small monomethyl alkanes.

L14 ANSWER 11 OF 37 CAPLUS COPYRIGHT 2003 ACS on STN DUPLICATE 1
ACCESSION NUMBER: 2001:229359 CAPLUS
DOCUMENT NUMBER: 134:353008
TITLE: A new 3D molecular structure representation using quantum topology with application to structure-property relationships
AUTHOR(S): Alsberg, Bjorn K.; Marchand-Geneste, Nathalie; King, Ross D.
CORPORATE SOURCE: The Computational Biology Group, Department of Computer Science, University of Wales, Ceredigion, SY23 3DB, UK
SOURCE: Chemometrics and Intelligent Laboratory Systems (2000), 54(2), 75-91
CODEN: CILSEN; ISSN: 0169-7439
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB We present a new 3D mol. structure representation based on Richard F.W. Bader's quantum topol. atoms in mols. (AIM) theory for use in quant. structure-property/activity relationship (**QSPR**/QSAR) modeling. Central to this structure representation using quantum topol. (StruQT) are crit. points located on the electron d. **distribution** of the mols. Other gradient fields such as the Laplacian of the electron d. **distribution** can also be used. The type of crit. point of particular interest is the bond crit. point (BCP) which is here characterized by using the following three parameters: electron d. .rho., the Laplacian 2.rho. and the ellipticity .epsilon.. This representation has the advantage that there is no need to probe a large no. of lattice points in 3D space to capture the important parts of the 3D electronic structure as is necessary in, e.g. comparative field anal. (CoMFA). We tested the new structure representation by predicting the wavelength of the lowest UV transition for a system of 18 anthocyanidins. Different quant. structure-property relationship (**QSPR**) models are constructed using several chemometric/machine learning methods such as std. partial least squares regression (PLS), truncated PLS variable selection, genetic algorithm-based variable selection and genetic programming (GP). These models identified bonds that either take part in decreasing or increasing the dominant excitation wavelength. The models also correctly emphasized on the involvement of the conjugated .pi. system for predicting the wavelength through flagging the BCP ellipticity parameters as important for this particular data set.

REFERENCE COUNT: 62 THERE ARE 62 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 12 OF 37 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2000:831791 CAPLUS
DOCUMENT NUMBER: 134:72809
TITLE: A review of QSAR for dye affinity for cellulose fibres
AUTHOR(S): Timofei, Simona; Schmidt, Walter; Kurunczi, Ludovic; Simon, Zeno
CORPORATE SOURCE: Institute of Chemistry, Romanian Academy, Timisoara, 1900, Rom.
SOURCE: Dyes and Pigments (2000), 47(1-2), 5-16
CODEN: DYPIDX; ISSN: 0143-7208
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English

AB A review with 101 refs. The structure of cellulose fiber is discussed in relation to the relevance of the ligand-receptor concept for dye-fiber binding. An outline of qual. SAR (structure-activity relationship) for dye-cellulose fiber binding is given, as well as of QSAR/**QSPR** (quant. structure-activity/property relationship) for such binding and calcns. of pertinent (electronic, geometric, and partition) properties of dye mols. Modern QSAR methods for dye-fiber **adsorption** include MTD (minimal steric difference) anal., CoMFA (comparative mol. field anal.), PCRA (principal component regression anal.), and neural network. Series of anthraquinone vat dyes, monoazo, disazo, and disperse dyes were studied by these methods. Conclusions from these QSAR studies concerning the effect of structural features of dye mols. upon **adsorption** on cellulose fibers are discussed.

REFERENCE COUNT: 101 THERE ARE 101 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 13 OF 37 MEDLINE on STN DUPLICATE 2
ACCESSION NUMBER: 2000315383 MEDLINE
DOCUMENT NUMBER: 20315383 PubMed ID: 10857384
TITLE: Caco-2 cell permeability vs human gastrointestinal absorption: **QSPR** analysis.
AUTHOR: Ren S; Lien E J
CORPORATE SOURCE: Department of Pharmaceutical Sciences, School of Pharmacy, University of Southern California, Los Angeles 90033, USA.
SOURCE: PROGRESS IN DRUG RESEARCH, (2000) 54 1-23.
Journal code: 1304021. ISSN: 0071-786X.
PUB. COUNTRY: Switzerland
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English
FILE SEGMENT: Priority Journals
ENTRY MONTH: 200006
ENTRY DATE: Entered STN: 20000706
Last Updated on STN: 20000706
Entered Medline: 20000629

AB The aim of this study is to elucidate quantitative structure-permeability relationship (**QSPR**) of various organic molecules through Caco-2 cells, and to ascertain the relationship between gastrointestinal (GI) absorption in humans and Caco-2 cell permeability. Caco-2 cell permeability and human GI absorption data were obtained from the literature. The maximum hydrogen bond-forming capacity corrected for intra-molecular H-bonding (Hbc) and Lien's QSAR model were used in this study. The latest CQSAR software was utilized in calculating the logarithm of partition coefficient in octanol/water (Clog P) and in deriving all regression equations. For 51 compounds, a significant correlation was obtained between Caco-2 cell permeability (log Pcaco-2) and Hbc, octanol/PBS (phosphate buffered saline, pH 7.4) **distribution** coefficient (log Doct), log MW and an indicator variable (I) for the charge, with a correlation coefficient of 0.797. When these compounds were divided into three subgroups, namely neutral, cationic and anionic compounds, much better correlations (r = 0.968, 0.915

and 0.931, respectively) were obtained using different combinations of various physico-chemical parameters. A plot of human GI absorption vs. Caco-2 cell permeability obtained from different laboratories reveals that Caco-2 cell permeability cannot be used to precisely predict human GI absorption for compounds with Pcaco-2 below 5 x 10(-6) cm/s, due to interlaboratory and experimental variabilities, and the lack of a simple correlation between human GI absorption and Caco-2 cell permeability. Caco-2 cell permeability may be estimated from the structures of drug molecules using the above-mentioned physicochemical parameters. In general, for compounds with Pcaco-2 above 5 x 10(-6) cm/s, human GI absorption ranges from 50 to 100%. This is generally acceptable for development into oral dosage form. For the compounds with Pcaco-2 below 5 x 10(-6) cm/s, careful interpretation of caco-2 cell permeability and use of internal standard for comparison are recommended. Otherwise, good drug candidates may be excluded due to incorrectly predicted poor absorption.

L14 ANSWER 14 OF 37 BIOSIS COPYRIGHT 2003 BIOLOGICAL ABSTRACTS INC. on STN
DUPLICATE 3

ACCESSION NUMBER: 2000:58837 BIOSIS
DOCUMENT NUMBER: PREV200000058837
TITLE: Quantitative structure-property relationship (**QSPR**) for the **adsorption** of organic compounds onto activated carbon cloth: Comparison between multiple linear regression and neural network.
AUTHOR(S): Brasquet, C. (1); Bourges, B.; Le Cloirec, P.
CORPORATE SOURCE: (1) Ecole des Mines de Nantes, DSEE, 44 307, Nantes Cedex 3 France
SOURCE: Environmental Science & Technology, (Dec. 1, 1999) Vol. 33, No. 23, pp. 4226-4231.
ISSN: 0013-936X.
DOCUMENT TYPE: Article
LANGUAGE: English
SUMMARY LANGUAGE: English

AB The **adsorption** of 55 organic compounds is carried out onto a recently discovered adsorbent, activated carbon cloth. Isotherms are modeled using the Freundlich classical model, and the large database generated allows qualitative assumptions about the **adsorption** mechanism. However, to confirm these assumptions, a quantitative structure-property relationship methodology is used to assess the correlation between an adsorbability parameter (expressed using the Freundlich parameter K) and topological indices related to the compounds molecular structure (molecular connectivity indices, MCI). This correlation is set up by mean of two different statistical tools, multiple linear regression (MLR) and neural network (NN). A principal component analysis is carried out to generate new and uncorrelated variables. It enables the relations between the MCI to be analyzed, but the multiple linear regression assessed using the principal components (PCs) has a poor statistical quality and introduces high order PCs, too inaccurate for an explanation of the **adsorption** mechanism. The correlations are thus set up using the original variables (MCI), and both statistical tools, multiple linear regression and neural network, are compared from a descriptive and predictive point of view. To compare the predictive ability of both methods, a test database of 10 organic compounds is used. Results show the good descriptive ability of NN compared with that of MLR, with more than 68% variance explained by NN, whereas MLR allows only 44% variance explanation. However, the predictive ability of NN seems to be low, especially when the structure of the test compounds is not well described in the training database. The good descriptive ability of NN is then exploited to carry out a variable analysis using the Garson weight partitioning method and to give information about the **adsorption** process. This study shows that flat molecules seem to be better adsorbed onto activated carbon fibers than bulky molecules, because of an **adsorption** which is located between the micrographitic planes of fibers. The **adsorption** process occurs via an electron

donor-acceptor interaction between the surface of the activated carbon fiber (donor) and the solute (acceptor). Consequently, the aromatic compounds with electron-withdrawing substituents seem to be favored. Furthermore, the lower the solute affinity for the aqueous media, the greater seems to be the **adsorption**.

L14 ANSWER 15 OF 37 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2000:276738 CAPLUS
DOCUMENT NUMBER: 133:88934
TITLE: Determination and **QSPR** analysis of log Kow and log Koc for fluorine containing benzene derivatives
AUTHOR(S): Yang, Hong; Tian, Chunrong; Li, Li; Han, Shuokui; Wang, Liansheng; Zhang, Zheng
CORPORATE SOURCE: Department of Environmental Science and Engineering, Nanjing University, Nanjing, 210093, Peop. Rep. China
SOURCE: Toxicological and Environmental Chemistry (1999), 69(3-4), 499-507
CODEN: TECSDY; ISSN: 0277-2248
PUBLISHER: Gordon & Breach Science Publishers
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Octanol-water partition coeffs. (Kow) and soil org. carbon sorption coeffs. (Koc) were detd. for 14 fluorinated benzene derivs. Quant. structure-property relationships were developed using mol. connectivity indexes and quantum chem. parameters to analyze the most significant factors influencing these physicochem. properties of the compds. The substitution by F in benzene derivs. has greater influence on Koc than on Kow.
REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 16 OF 37 MEDLINE on STN
ACCESSION NUMBER: 1999139102 MEDLINE
DOCUMENT NUMBER: 99139102 PubMed ID: 9971916
TITLE: Investigation of the mechanism of flux across human skin in vitro by quantitative structure-permeability relationships.
COMMENT: Comment in: Eur J Pharm Sci. 2001 Oct;14(3):197-200
Comment in: Eur J Pharm Sci. 2002 Jun;15(5):399-403
AUTHOR: Cronin M T; Dearden J C; Moss G P; Murray-Dickson G
CORPORATE SOURCE: School of Pharmacy and Chemistry, Liverpool John Moores University, Byrom Street, Liverpool L3 3AF, UK.. m.t.cronin@livjm.ac.uk
SOURCE: EUROPEAN JOURNAL OF PHARMACEUTICAL SCIENCES, (1999 Mar) 7 (4) 325-30.
Journal code: 9317982. ISSN: 0928-0987.
PUB. COUNTRY: Netherlands
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English
FILE SEGMENT: Priority Journals
ENTRY MONTH: 199904
ENTRY DATE: Entered STN: 19990426
Last Updated on STN: 20030102
Entered Medline: 19990413
AB Permeability coefficients for 114 compounds across excised human skin in vitro were taken from Kirchner et al. Forty-seven descriptors were calculated encompassing the relevant physicochemical parameters of the compounds. Quantitative structure-permeability relationships (QSPRs) were developed using least-squares regression analysis. A two-parameter **QSPR**, describing the permeability coefficients (Kp) across excised skin, was obtained: log Kp=0.772 log P -0.0103 Mr - 2.33 where log P is the logarithm of the octanol-water partition coefficient and Mr is molecular mass. This equation indicates that percutaneous absorption is mediated by the hydrophobicity and the molecular size of the penetrant.

Comparison with a **QSPR** based on penetration across a synthetic (polydimethylsiloxane) membrane suggests that the mechanisms of drug flux across polydimethylsiloxane membranes and excised human skin are significantly different.

L14 ANSWER 17 OF 37 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1999:158443 CAPLUS
DOCUMENT NUMBER: 130:281906
TITLE: Solvent extraction and **QSPR** of catecholamines with a bis(2-ethylhexyl) hydrogen phosphate
AUTHOR(S): Yoshizuka, Kazuharu; Fujimoto, Yuko; Ohto, Keisuke; Inoue, Katsutoshi
CORPORATE SOURCE: Department of Applied Chemistry, Saga University, Saga, 840-8502, Japan
SOURCE: Journal of Chemical Engineering of Japan (1999), 32(1), 76-81
CODEN: JCEJAQ; ISSN: 0021-9592
PUBLISHER: Society of Chemical Engineers, Japan
DOCUMENT TYPE: Journal
LANGUAGE: English
AB In order to develop an effective sepn. process for catecholamine (CA), a basic investigation on solvent extn. of dopamine (DA), adrenaline (Ad) and noradrenaline (NA) from hydrochloric acid soln. and their stripping is conducted at 30.degree.C employing bis(2-ethylhexyl) hydrogen phosphate (D2EHPA) in chloroform, n-hexane and toluene as the org. diluents. From the dependencies of the **distribution** ratios on the concns. of reactant species, i.e. CA, hydrogen ion and D2EHPA, it is elucidated that CA (RNH2) is extd. with D2EHPA (HR') according to the ion exchange mechanism, as the complex type, RNH3R'(HR')3, and the equil. consts. (Kex,CA) for the extn. reactions are also evaluated. The quant. structure property relationship (**QSPR**) of Kex,CA values for each org. diluent is discussed using mol. modeling with semi-empirical MO calcns. considering the solvent effect.
REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 18 OF 37 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2000:841246 CAPLUS
DOCUMENT NUMBER: 134:71021
TITLE: Using AM1 hamiltonian in prediction of benzaldehydes sorption on soil
AUTHOR(S): Jin, Lijun; Guo, Pan; Wang, Liansheng; Wei, Zhongbo; Zhang, Zheng
CORPORATE SOURCE: State Key Laboratory of Pollution Control and Resource Reuse, Department of Environmental Science and Engineering, Nanjing University, Nanjing, 210093, Peop. Rep. China
SOURCE: Toxicological and Environmental Chemistry (1998), 67(3-4), 471-479
CODEN: TECSDY; ISSN: 0277-2248
PUBLISHER: Gordon & Breach Science Publishers
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The sorption behavior of 15 substituted benzaldehydes on natural soil has been reported. It was found that most of the sorption isotherms were nonlinear, log Kf correlated poorly with log Kow and log Sw. Descriptors derived from quantum computation were used to develop a **QSPR** model, which could be used to predict the log Kf of similar compds. This study showed that the gap (.DELTA.E) between the energy of the LUMO and the energy of the HOMO was the principle factor controlling the sorption behavior of tested chems. Other important variables contained the most pos. net at. charge on an atom (q+) and final heat of formation (HF). This shows that chemisorption and phys. **adsorption** may be the

fundamental process for benzaldehydes sorption on natural soil other than lipophilic partitioning.
REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 19 OF 37 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1998:460441 CAPLUS
DOCUMENT NUMBER: 129:235856
TITLE: Improved valence connectivity topological index and its application - .delta.i- comparison with .delta.v in QSAR/**QSPR** of three systems
AUTHOR(S): Yang, Feng; Yan, Xiaoci; Ouyang, Li; Wang, Liya; Luo, Mingdao; Wang, Tainzhi; Qu, Songsheng
CORPORATE SOURCE: Department Chemistry, Wuhan University, Wuhan, 430072, Peop. Rep. China
SOURCE: Huaxue Wuli Xuebao (1998), 11(3), 221-226
CODEN: HWXUE4; ISSN: 1003-7713
PUBLISHER: Zhongguo Kexue Jishu Daxue Chubanshe
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
AB The valence connectivity index .delta.v is not suitable for the inorg. compds. which have complicated oxidn. state (for example, Si+, Si2+, Si3+, Si4+) and the org. compds. which include many types of heteroatoms such as F, Cl, Br, I, O, S, etc., in order to enlarge the fields of .delta.v, on the basis of .delta.v, the authors defined the valence connectivity index .delta.i-, by introducing the main quantum no., the no. of valence electrons to the atom under study. The improved mol. topol. index 1X- was defined by means of .delta.i-. The X0- of SiXn (n=1 .apprx. 4, X = F, Cl, Br, I), the 1X- of ClmSi(OR)n (m+n=4) and halo benzenes were calcd. The linear relations of X0- and the .delta.fHm of SiXn, 1X- and the GC retention index (RI) of ClmSi(OR)n, 1X- and the soly. S and the **distribution** coeff. P (octanol/water) of halo benzenes are good, their correlation coeffs. R are 0.9928, 0.97, 0.9694, 0.99929, resp. The results are much better than those of the topol. indexes X0v and Xv which are detd. by .delta.v (the correlation coeffs. are 0.8862, 0.70, 0.9131, 0.9387, correspondingly).

L14 ANSWER 20 OF 37 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1998:139270 CAPLUS
TITLE: Evaluation and use of BCUT descriptors in QSAR and **QSPR** studies.
AUTHOR(S): Stanton, David T.
CORPORATE SOURCE: Procter and Gamble Pharmaceuticals, Mason, OH, 45040-9662, USA
SOURCE: Book of Abstracts, 215th ACS National Meeting, Dallas, March 29-April 2 (1998), COMP-073. American Chemical Society: Washington, D. C.
CODEN: 65QTAA
DOCUMENT TYPE: Conference; Meeting Abstract
LANGUAGE: English
AB BCUT descriptors were originally developed for use as structural descriptors in diversity anal. applications. These descriptors capture the details of structural features relating to hydrogen bond donating and accepting ability, polarizability, and charge **distribution**. Such features are responsible for the strong electrostatic and polar interactions between mols. Because of this, the BCUT descriptors provide information that is not readily available using other typical structural descriptors, and have been found to complement QSAR descriptors that focus more on structural features responsible for non-polar and hydrophobic interactions. We have found that they contribute significantly to QSAR models of data sets where polar interactions are important. Examples will be provided that illustrate their utility in both QSAR and **QSPR** model development applications.

L14 ANSWER 21 OF 37 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1998:225034 CAPLUS
DOCUMENT NUMBER: 129:4416
TITLE: Quantitative structure-retention relationship study of tetrazolium salts on alumina support
AUTHOR(S): Cserhati, Tibor; Kosa, Agnes; Balogh, Sandor
CORPORATE SOURCE: Central Research Institute for Chemistry, Hungarian Academy of Sciences, Budapest, 1525, Hung.
SOURCE: Biomedical Chromatography (1998), 12(2), 61-64
CODEN: BICHE2; ISSN: 0269-3879
PUBLISHER: John Wiley & Sons Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The retention of 7 monotetrazolium and 9 ditetrazolium salts was detd. on alumina and reversed-phase (RP) alumina layers using n-hexane-2-propanol and water-2-propanol mixts. as eluents. The retention capacity and the sp. surface area of solutes in contact with the stationary phases were calcd. Quant. structure-retention relationship calcns. indicated that the retention capacity of solutes on RP alumina layers depended not only on the mol. hydrophobicity but also on the hydrogen-donor and acceptor properties. Sp. surface areas were related to the electronic and steric parameters of the solutes. Calcns. suggested that the retention on both alumina and RP alumina layers is of mixed character, hydrophobic, electronic and steric parameters are equally involved in the retention.
REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 22 OF 37 CAPLUS COPYRIGHT 2003 ACS on STN DUPLICATE 4
ACCESSION NUMBER: 1998:302689 CAPLUS
DOCUMENT NUMBER: 129:31413
TITLE: 3D-modeling and prediction by WHIM descriptors. Part 9. Chromatographic relative retention time and physico-chemical properties of polychlorinated biphenyls (PCBs)
AUTHOR(S): Gramatica, P.; Navas, N.; Todeschini, R.
CORPORATE SOURCE: Department of Environmental Sciences, University of Milan, Milan, I-20126, Italy
SOURCE: Chemometrics and Intelligent Laboratory Systems (1998), 40(1), 53-63
CODEN: CILSEN; ISSN: 0169-7439
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Physicochem. properties of polychlorinated biphenyl (PCB) congeners have been extensively studied searching for quant. structure-property relationships (**QSPR**). Chem. descriptions of PCB structure are made in terms of WHIM descriptors, i.e., 3-dimensional mol. descriptors which account for size, shape, symmetry, and atom **distribution** of the mols. Regression models have been obtained by optimizing their predictive power and selecting the best subset of descriptors by genetic algorithm. Results confirmed the capability of this approach to give predictive models for important physicochem. properties, such as relative retention time, log Kow, m.p., total surface area, Henry's law const., soly., and aq. activity coeffs.
REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 23 OF 37 BIOSIS COPYRIGHT 2003 BIOLOGICAL ABSTRACTS INC. on STN
ACCESSION NUMBER: 1998:105374 BIOSIS
DOCUMENT NUMBER: PREV199800105374
TITLE: Quantitative structure property relationships (**QSPR**) for prediction of solution **adsorption** process parameters using fumed silica.
AUTHOR(S): Wang, Lily; Matheson, Lloyd E.

CORPORATE SOURCE: Coll. Pharm., Univ. Iowa, Iowa City, IA 52242 USA
SOURCE: Pharmaceutical Research (New York), (Nov., 1997) Vol. 14, No. 11 SUPPL., pp. S483.
Meeting Info.: Annual Meeting of the American Association of Pharmaceutical Scientists Boston, Massachusetts, USA November 2-6, 1997 American Association of Pharmaceutical Scientists
. ISSN: 0724-8741.
DOCUMENT TYPE: Conference
LANGUAGE: English

L14 ANSWER 24 OF 37 EMBASE COPYRIGHT 2003 ELSEVIER INC. ALL RIGHTS RESERVED. on STN
ACCESSION NUMBER: 96167762 EMBASE
DOCUMENT NUMBER: 1996167762
TITLE: Prediction of the soil sorption coefficient of organic pollutants by the characteristic root index model.
AUTHOR: Sacan M.T.; Balcioglu I.A.
CORPORATE SOURCE: Istanbul University, Faculty of Science, Department of Biology 34459,Vezneciler, Istanbul, Turkey
SOURCE: Chemosphere, (1996) 32/10 (1993-2001).
ISSN: 0045-6535 CODEN: CMSHAF
COUNTRY: United Kingdom
DOCUMENT TYPE: Journal; Article
FILE SEGMENT: 046 Environmental Health and Pollution Control
LANGUAGE: English
SUMMARY LANGUAGE: English
AB Quantitative Structure-Property Relationship (**QSPR**) technique was used to develop a simple predictive model for the soil sorption coefficient (K(oc)) of Polychlorinated Biphenyls (PCBs), chlorinated phenols (CPs) and chlorinated benzenes (CBs). Tests performed on 36 such compounds clearly demonstrate that this simple model accurately predicts, the soil sorption coefficients of these chemicals. The correlation equation was then used to predict the unknown soil sorption data of chlorinated biphenyls, phenols and benzenes. The result of these tests also demonstrates that the CRI can be an alternative and a very accurate predictive tool for the soil sorption coefficients of structurally similar compounds.

L14 ANSWER 25 OF 37 BIOSIS COPYRIGHT 2003 BIOLOGICAL ABSTRACTS INC. on STN DUPLICATE 5
ACCESSION NUMBER: 1996:419859 BIOSIS
DOCUMENT NUMBER: PREV199699142215
TITLE: **Adsorption** behaviour and **QSPR** studies of organotin compounds on estuarine sediment.
AUTHOR(S): Sun, Hongwen; Huang, Guolan; Dai, Shugui
CORPORATE SOURCE: Dep. Environ. Sci., Nankai Univ., Tianjin 300071 China
SOURCE: Chemosphere, (1996) Vol. 33, No. 5, pp. 831-838.
ISSN: 0045-6535.
DOCUMENT TYPE: Article
LANGUAGE: English
AB The **adsorption** behaviour of eight organotin species and Sn-4+ (SnCl-4) on estuarine sediments has been reported for the first time. It was found that the **adsorption** of organotins varies greatly with molecular structure. The order of **adsorption** coefficient k is Sn-4+ gt mono- gt di- gt tri-organotins. Correlations or log k with eight different structural parameters show that the electronic properties of the Sn atom is the principal factor controlling the **adsorption** behaviour of organotins. The **adsorption** mechanism of organotins is mainly an ion-exchange process, with little lipophilic partitioning.

L14 ANSWER 26 OF 37 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1996:219060 CAPLUS
TITLE: Use of semiempirical quantum-chemical molecular

descriptors in QSAR **QSPR**.
AUTHOR(S): Karelson, Mati
CORPORATE SOURCE: Department Chemistry, University Tartu, Tartu, EE2400, Estonia
SOURCE: Book of Abstracts, 211th ACS National Meeting, New Orleans, LA, March 24-28 (1996), COMP-154. American Chemical Society: Washington, D. C.
CODEN: 62PIAJ
DOCUMENT TYPE: Conference; Meeting Abstract
LANGUAGE: English
AB Modern semiempirical quantum-chem. methods allow calcn. of numerous mol. characteristics (descriptors) which can be efficiently used in the development of quant. structure activity property relationships (QSAR **QSPR**). These characteristics are calcd. mostly on the basis of the electronic wavefunction and charge **distribution** and include the partial at. charges, partial charged (solvent-accessible) surface areas, frontier MO energies, mol. elec. moments and their components, Fukui reactivity indexes, various electronic-topol. descriptors etc. The Comprehensive Descriptors for Structural and Statistical Anal. (CODESSA) approach and software have been successfully applied to describe phys. properties (b.p., m.p., etc.), biol. activity, and chem. reactivity of a large variety of org. and inorg. compds., using the quantum-chem. developed descriptors and their combination with the conventional geometrical and topol. mol. descriptors. In most cases, the correlation equations developed have given addnl. valuable information about the phys. mechanism of interaction involved in the phenomenon or process studied.

L14 ANSWER 27 OF 37 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1997:223596 CAPLUS
DOCUMENT NUMBER: 126:263718
TITLE: Rotational barrier of the polychlorinated biphenyls as a physicochemical parameter for use in modeling of QSARs and QSPRs
AUTHOR(S): Andersson, Patrik L.; Haglund, Peter; Tysklind, Mats
CORPORATE SOURCE: Institute Environmental Chemistry, Umea University, Umea, S-90187, Swed.
SOURCE: Organohalogen Compounds (1996), 28, 47-52
CODEN: ORCOEP
PUBLISHER: ECO-INFORMA Press
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Internal rotation barriers of PCBs were calcd. to 2.0-115.5 kcal/mol. It is shown that the **distribution** coeff. and the vapor pressure of PCBs are related to the internal barrier of rotation. Addnl., a correlation was found between the rotational barrier and the inhibition of intercellular communication.

L14 ANSWER 28 OF 37 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1995:508238 CAPLUS
DOCUMENT NUMBER: 122:248923
TITLE: **QSPR** and GCA Models for Predicting the Normal Boiling Points of Fluorocarbons
AUTHOR(S): Le, Thao D.; Weers, Jeffry G.
CORPORATE SOURCE: Alliance Pharmaceutical Corporation, San Diego, CA, 92121, USA
SOURCE: Journal of Physical Chemistry (1995), 99(17), 6739-47
CODEN: JPCHAX; ISSN: 0022-3654
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Quant. structure-property relationship (**QSPR**) and group contribution-additivity (GCA) models have been developed for predicting the normal b.ps. of diverse fluorocarbons and fluorocarbon-hydrocarbon diblock compds. The models are based on exptl. b.ps. and intrinsic mol.

properties (i.e., dynamic polarizability and isopotential surfaces) of 68 uniquely structured fluorocarbons. The mol. properties were obtained from quantum mech. calcns. utilizing the PM3 Hamiltonian. The **QSPR** and GCA models have an av. error of 5 and 3%, resp. The error redn. in the GCA model is due to effective **distribution** of the contributory propagated errors. A wide range of fluorocarbons was examd., and 21 group contributions were delineated. These include such groups and heteroatoms as RF, RH, C:O, NH2, OH, C, N, O, Cl, Br, and I.

L14 ANSWER 29 OF 37 BIOSIS COPYRIGHT 2003 BIOLOGICAL ABSTRACTS INC. on STN
DUPLICATE 6
ACCESSION NUMBER: 1995:397862 BIOSIS
DOCUMENT NUMBER: PREV199598412162
TITLE: Quantitative structure-pharmacokinetics relationships (**QSPR**) of beta blockers derived using neural networks.
AUTHOR(S): Gobburu, Jogarao V. S.; Shelver, William H. (1)
CORPORATE SOURCE: (1) Dep. Pharm. Sci., North Dakota State Univ., Fargo, ND 58105 USA
SOURCE: Journal of Pharmaceutical Sciences, (1995) Vol. 84, No. 7, pp. 862-865.
ISSN: 0022-3549.
DOCUMENT TYPE: Article
LANGUAGE: English
AB This study demonstrates the application of neural networks to predict the pharmacokinetic properties of beta-adrenoreceptor antagonists in humans. A congeneric series of 10 beta-blockers, whose critical pharmacokinetic parameters are well established, was selected for the study. An appropriate neural network system was constructed and tested for its ability to predict the pharmacokinetic parameters from the octanol/ water partition coefficient (shake flask method), the pK-a, or the fraction bound to plasma proteins. Neural networks successfully trained and the predicted pharmacokinetic values agreed well with the experimental values (average difference = 8%). The neural network-predicted values showed better agreement with the experimental values than those predicted by multiple regression techniques (average difference = 47%). Because the neural networks had a large number of connections, two tests were conducted to determine if the networks were memorizing rather than generalizing. The "leave-one-out" method verified the generalization of the networks by demonstrating that any of the compounds could be deleted from the training set and its value correctly predicted by the new network (average error = 19%). The second test involved the prediction of pharmacokinetic properties of compounds never seen by the network, and reasonable results were obtained for three out of four compounds tested. The results indicate neural networks can be a powerful tool in exploration of quantitative structure-pharmacokinetic relationships.

L14 ANSWER 30 OF 37 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1996:10286 CAPLUS
DOCUMENT NUMBER: 124:98458
TITLE: Prediction of surface tension of organic liquids
AUTHOR(S): Kavun, S. M.; Chalykh, A. E.; Palyulin, V. A.
CORPORATE SOURCE: Tire Industry Research Inst., Moscow, 105118, Russia
SOURCE: Colloid Journal (Translation of Kolloidnyi Zhurnal) (1995), 57(6), 767-71
CODEN: CJRSEQ; ISSN: 1061-933X
PUBLISHER: MAIK Nauka/Interperiodica
DOCUMENT TYPE: Journal
LANGUAGE: English
AB With the use of **QSPR** procedure, graph theory and several techniques of phys. and theor. org. chem., a simple quant. regression equation was derived making it possible to predict values of surface tension .sigma. of liq. org. compds. of various classes with good accuracy. In this equation, three blocks of descriptors were used

characterizing charge **distribution** on atoms of mols., a ratio between polar and apolar van der Waals surface areas, and branching of mols. It was noted that the values of surface tension correlate poorly with each single descriptor, thus, indicating a fine balance between descriptor contributions in the equation derived and their complex involvement in the description of .sigma..

L14 ANSWER 31 OF 37 BIOSIS COPYRIGHT 2003 BIOLOGICAL ABSTRACTS INC. on STN
ACCESSION NUMBER: 1995:319597 BIOSIS
DOCUMENT NUMBER: PREV199598333897
TITLE: **QSPR** and QSAR study of phthalimidohydroxamic acids.
AUTHOR(S): Nikolic, Sonja (1); Medic-Saric, Marica; Matijevic-Sosa, Julija
CORPORATE SOURCE: (1) Rugjer Boskovic Inst., PO Box 1016, HR-41001 Zagreb Croatia
SOURCE: Acta Pharmaceutica (Zagreb), (1995) Vol. 45, No. 1, pp. 15-24.
ISSN: 0354-2971.
DOCUMENT TYPE: Article
LANGUAGE: English
SUMMARY LANGUAGE: English; Serbo-Croatian
AB Newly prepared phthalimidohydroxamic acids are tested for their mitodepressive effect on the growth of Lepidium sativum L. seeds (Cresson). Their partition coefficients, log P(o/w), are calculated by Rekker method. In the structure-property-activity study we have used topological indices to predict the physico-chemical properties and bioactivity of the prepared compounds. The optimal **QSPR** and QSAR models are obtained by using the valence connectivity index and the information-theoretic index.

L14 ANSWER 32 OF 37 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1995:920429 CAPLUS
TITLE: Theory and software for a general model of solute-solvent interactions.
AUTHOR(S): Brusniak, Mi-Youn K.; Smith, Karl M.; Escobar, Jose-Luis; Balducci, Renzo; Deanda, Felix; Pearlman, Robert S.
CORPORATE SOURCE: College Pharmacy, University Texas, Austin, TX, 78712, USA
SOURCE: Book of Abstracts, 210th ACS National Meeting, Chicago, IL, August 20-24 (1995), Issue Pt. 1, ENVR-005. American Chemical Society: Washington, D. C.
CODEN: 61XGAC
DOCUMENT TYPE: Conference; Meeting Abstract
LANGUAGE: English
AB Soln.-phase properties such as partition coeff., permeability coeff., and free energy of desolvation (needed for modeling **adsorption** coeffs. or protein--ligand binding consts.) can be modeled in terms of one or more gas-to-soln. transfer processes. Each gas-to-soln. transfer process is modeled in terms of the free energy of cavity formation and the free energy of solute-solvent interaction. We will briefly review our general model for the calcn. of the various components of these free energies. In particular, we will present a novel approach to the estn. of the conformational (i.e., bond-rotational) entropy loss which accompanies gas-to-soln. or soln.-to-"solid" transfer. By considering both the rotational energy barriers and the "rotational damping" due to the viscosity of the solute environment, this novel model has proven to be significantly more useful than simply counting the no. of "rotatable" bonds. We will conclude by summarizing the various software components developed in order to implement the general solvation model and to provide addnl. chem. descriptors useful for **QSPR** purposes.

L14 ANSWER 33 OF 37 BIOSIS COPYRIGHT 2003 BIOLOGICAL ABSTRACTS INC. on STN
ACCESSION NUMBER: 1993:503792 BIOSIS
DOCUMENT NUMBER: PREV199396127799
TITLE: A comparative study of some topological indices and log P in structure-property-activity analysis of phenylalkylamines.
AUTHOR(S): Medic-Saric, M. (1); Rendic, S.; Vestemar, V.; Saric, S.
CORPORATE SOURCE: (1) Dep. Pharmaceutical Chem., Fac. Pharm. and Biochem., Univ. Zagreb, 41000 Zagreb, The Republic of Croatia
SOURCE: Acta Pharmaceutica Zagreb, (1993) Vol. 43, No. 1, pp. 15-26.
DOCUMENT TYPE: Article
LANGUAGE: English
SUMMARY LANGUAGE: English; Serbo-Croatian
AB Physico-chemical properties (lipophilicity - log P and molecular mass - M.m.) and biological activity (norepinephrine-uptake inhibition - log A) of phenylalkylamines were quantitatively analyzed. Topological indices used for correlation analysis include Wiener's number, Randic connectivity index, Balaban's index and information-theoretic index. The comparison of four topological indices shows that Wiener's number is the most convenient as the structural parameter in quantitative structure-property relationship (**QSPR**), as well as in quantitative structure-activity relationship (QSAR) analysis of phenylalkylamines. A number of indices, except Randic connectivity index, are found to be equieffective or superior to log P in correlations with biological activity.

L14 ANSWER 34 OF 37 CAPLUS COPYRIGHT 2003 ACS on STN DUPLICATE 7
ACCESSION NUMBER: 1992:127606 CAPLUS
DOCUMENT NUMBER: 116:127606
TITLE: Predictive **QSPR** models for estimating soil sorption coefficients: potential and limitations based on dominating processes
AUTHOR(S): Von Oepen, B.; Koerdel, W.; Klein, W.; Schueuermann, G.
CORPORATE SOURCE: Fraunhofer-Inst. Umweltchem. Oekotoxikol., Schmallenberg, D-5948, Germany
SOURCE: Science of the Total Environment (1991), 109-110, 343-54
CODEN: STENDL; ISSN: 0048-9697
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The sorption coeffs. of 50 org. chems. and pesticides of defined chem. classes (carboxylic acids, esters, amines, and amides - polar and nonpolar) were detd. with 3 different sorbents (Alfisol, Podzol, and sediment) according to OECD Guideline 106. For various xenobiotics, the potential of predicting Koc from mol. descriptors, e.g. electronic, geometric (calcd. by quantum mech. methods) and topol. parameters, was analyzed to det. the scope and limitations of resp. quantum structure-property relationships. Several regression equations were derived for nonpolar compds., e.g. esters. For the more polar compds., the variation in Koc values was .ltoreq.2 orders of magnitude, and only poor correlations were obtained for most of the descriptors studied.

L14 ANSWER 35 OF 37 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1991:505433 CAPLUS
DOCUMENT NUMBER: 115:105433
TITLE: Quantitative structure - pharmacokinetic relationship (**QSPR**) analysis for arylalkanoic acid nonsteroidal anti-inflammatory drugs
AUTHOR(S): Dhake, A. S.; Patvardhan, P. D.; Tipnis, H. P.
CORPORATE SOURCE: Bombay Coll. Pharm., Bombay, 400 098, India
SOURCE: Indian Drugs (1991), 28(7), 291-6
CODEN: INDRBA; ISSN: 0019-462X

DOCUMENT TYPE: Journal
LANGUAGE: English
AB **QSPR** enables to predict the pharmacokinetic properties of compds. before their synthesis and leads to a rational design of new drugs. Nine members belonging to the arylalkanoic acid series of NSAIDs were selected for studying the quant. relationship of pharmacokinetic parameters to mol. structure. Hansch method was used for **QSPR** anal. The disposition parameters-apparent vol. of **distribution**, apparent clearance and elimination half-life, in human volunteers were considered for this study. The variation of these parameters with the structural parameters, log P, pKa and mol. connectivity indexes has been discussed.

L14 ANSWER 36 OF 37 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1993:6407 CAPLUS
DOCUMENT NUMBER: 118:6407
TITLE: General methodology and computer program for the exhaustive restoring of chemical structures by molecular connectivity indexes. Solution of the inverse problem in QSAR/**QSPR**
AUTHOR(S): Gordeeva, E. V.; Molchanova, M. S.; Zefirov, N. S.
CORPORATE SOURCE: N. D. Zelinskii Inst. Org. Chem., Moscow, 117913, Russia
SOURCE: Tetrahedron Computer Methodology (1990), 3(6B), 389-415
CODEN: TCMTE6; ISSN: 0898-5529
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The first attempt to attack an intriguing inverse problem in QSAR/**QSPR** is presented. The special technique to the exhaustive targeted search of the structures with a given value of mol. connectivity index is described. The general methodol. and the combinatorial algorithm are considered. The selection criteria for the correct generation of graphs and multigraphs with the given **distribution** of edge types or vertex types are developed. The RING program for the exhaustive generation of structures with the given connectivity index is described, and several examples of its successful application are discussed. A demo version of RING is included in this issue.

L14 ANSWER 37 OF 37 MEDLINE on STN
ACCESSION NUMBER: 86055667 MEDLINE
DOCUMENT NUMBER: 86055667 PubMed ID: 3905378
TITLE: Development of quantitative structure-pharmacokinetic relationships.
AUTHOR: Mayer J M; van de Waterbeemd H
SOURCE: ENVIRONMENTAL HEALTH PERSPECTIVES, (1985 Sep) 61 295-306.
Ref: 122
Journal code: 0330411. ISSN: 0091-6765.
PUB. COUNTRY: United States
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
General Review; (REVIEW)
LANGUAGE: English
FILE SEGMENT: Priority Journals
ENTRY MONTH: 198601
ENTRY DATE: Entered STN: 19900321
Last Updated on STN: 19980206
Entered Medline: 19860115
AB Quantitative structure-activity relationships (QSAR) relating biological activity to physiochemical descriptors have been successfully used for a number of years. It is also long recognized that pharmacokinetic parameters may play an important and even determinant role in drug action. This prompted several researchers to focus attention to pharmacokinetic parameters as potential descriptors in quantitative drug design. A number of examples of quantitative structure-pharmacokinetic relationships (

QSPR) have appeared in the literature. The present contribution reviews some developments in this field. In particular, a number of concepts and problems are critically discussed, rather than compilations of examples already published in recent reviews. Attention will be paid to the main processes of the pharmacokinetic or toxicokinetic phase in drug action, including absorption, **distribution** and elimination (biotransformation and excretion). It is clear that quantitative approaches are of considerable interest to toxicologists, since these methods may contribute to the development of real predictive toxicology.

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